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Title: **Quantum imitations of physical phenomena**

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Quantum imitations of physical phenomena*

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Abstract

Quantum imitation is an attempt to exploit quantum laws to advantage, and thus accomplish efficient simulation of physical phenomena. We discuss the fundamental concepts behind this new paradigm of information processing, such as the connection between models of computation and physical systems, along with the first imitation of a toy quantum many-body problem.

1 Introduction

Recently, a new paradigm in Information Theory and Computer Science has emerged as a result of the application of the fundamental laws that govern our real physical universe, i.e., Quantum Mechanics. Information is fungible and physically realizable and, therefore, subjected to the laws of physics that place limits on computation [1]. The close connection between information processing and its physical realization is perhaps one of the most remarkable aspects of this new paradigm whose set of ideas constitute what is currently known as "Quantum Information and Computation" [2]; the device that performs such manipulation of information is named "quantum computer" (QC) and a fundamental unit of computation is the quantum bit or *qubit* (a quantum two-level system).

In this way quantum computation represents a paradigm for information processing that makes use of the laws of Quantum Mechanics and, as such, is in principle independent of the particular experimental realization of the QC. Indeed, in the following I will assume that a QC exists (i.e., I

*Different aspects of this work were done in collaboration with J.E. Gubernatis, E. Knill, R. Laflamme, C. Negrevergne and R. Somma.

will not discuss the important problem of quantum noise or decoherence) and a natural question to address is what can be done with such a device that cannot be done efficiently with a classical computer (CC) (either probabilistic or deterministic)? In this regard, the problem of simulating physical phenomena and, in particular, studying the properties of matter at very low temperatures is an obvious candidate since they are believed to be problems with exponential complexity (both in space and time).

On a deterministic CC the difficulty is associated with the number of resources needed to describe a quantum system, growing exponentially with the size of the system. In other words, *Hilbert space is too large*. On a probabilistic CC the situation is less clear [3, 4]. A particular class of such problems deserving special attention are the fermionic ones. We all know that the bottleneck with simulating fermionic systems on a probabilistic CC is the infamous sign problem which makes the simulation exponentially hard. One would like to know, for example, whether a QC reduces its complexity to polynomial and we will see that this is case for certain sign problems.

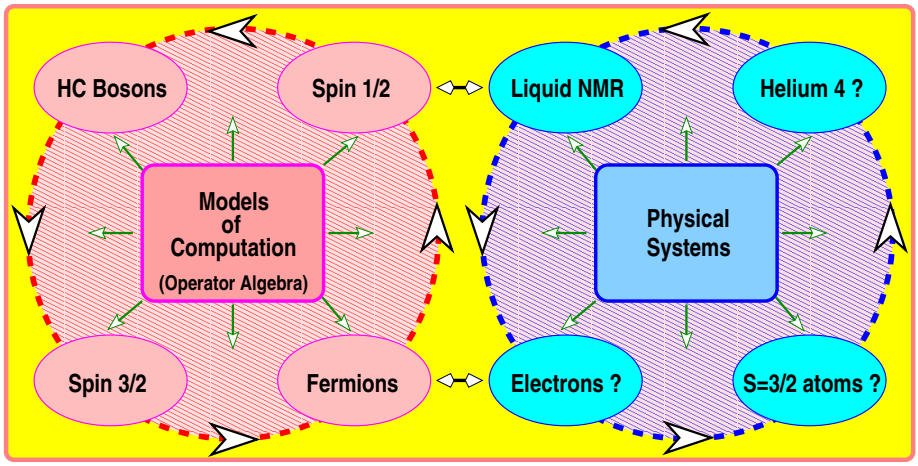

Figure 1: Relationship between different models of computation (with their associated operator algebras) and different physical systems. Question marks refer to the present lack of a QC device using the corresponding elementary physical components indicated in the box. Diamond-shaped arrows represent the natural connection between physical system and operator language, while arrows on the circle indicate the existence of isomorphisms of $*$-algebras, therefore, the corresponding simulation of one physical system by another.

To be useful as a physics simulation device, a QC must answer questions about physical properties associated with real physical systems. These questions are often concerned with the expectation values of specific measurements of a quantum state evolved from a specific initial state. Consequently, the initialization, evolution, and measurement processes must all be implementable with polynomial scaling [3]. Often it is difficult to do. Further, some classes of measurements, such as thermodynamic ones, still lack well-defined workable algorithms. The hope is, however, that quantum imitation is "more" efficient (less resources) than classical simulation and there are examples that support such hope [3, 5].

2 Quantum Imitation of Physical Phenomena

Following Sections will introduce some of the most relevant concepts to accomplish efficient quantum imitation of physical phenomena. [1]

2.1 Models of Computation and Physical Systems

A fundamental concept in quantum information processing is the connection of a quantum computational model to a physical system by transformations of closed operator algebras. The concept is a necessary one because in Quantum Mechanics each physical system is naturally associated with a language of operators (for example, quantum spin-1/2 operators) and thus to an algebra realizing this language (e.g., the Pauli spin algebra generated by commuting quantum spin-1/2 operators). Any quantum system defined by an algebra of operators generated by a set of "basic" operators can be considered as a possible model of quantum computation [3]. The remarkable fact is that an arbitrary physical system is simulatable by another physical system (or QC) whenever isomorphic mappings (embeddings) between the two operator algebras exists. In each such case, an important problem is to determine whether the simulation is efficient (polynomial resource overhead) in terms of the "basic" generators. For example, a nuclear spin (NMR) QC is modeled as a collection of quantum spin-1/2 objects and described by the Pauli algebra. It can simulate a system of ^{4}He atoms (with space discretized by a lattice) represented by

[1] Some ideas and examples described in the present Note have already appeared in earlier work [3, 5].

the hard-core bosonic algebra, and vice versa. In this case, the simulation is efficient. Figure 1 summarizes this fundamental concept by giving a variety of proposed physical models for QCs and associated usable operator algebras. If one of these systems suffices as the universal model of quantum computing, the mappings between the operator algebras establish the equivalence of the other physical models to it. This is one's intuitive expectation, and has a well-established mathematical basis [6].

A model of quantum computation requires physical systems that can be controlled by modulating the parameters of the system's Hamiltonian (quantum control). The method for defining a model of quantum computation consists of giving an algebra of operators with a set of controllable Hamiltonians (Hermitian operators in the algebra), a set of measurable observables, and an initial state of the physical system. In physical terms, specifying a model of computation amounts to respond the following questions: What is the state space?, What is the initial state?, How can states be manipulated? and How do we get information about a state?

In the standard model of quantum computation, the qubit is the fundamental unit. A qubit's state $|\varphi\rangle$ is a linear combination of the states $|0\rangle$ and $|1\rangle$ (e.g, a spin 1/2 with $|0\rangle = |\uparrow\rangle,\ |1\rangle = |\downarrow\rangle$):

$$|\varphi\rangle = a\ |0\rangle + b\ |1\rangle\ ,$$

where the complex numbers a and b are normalized to unity: $|a|^2+|b|^2 = 1$.

Assigned to each qubit are the identity matrix $\mathbb{1}$ and the Pauli matrices

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\ ,\ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\ ,\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\ ,\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\ ,$$

or equivalently $\mathbb{1}$, $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$, and σ_z. In this particular representation, the states $|0\rangle$ and $|1\rangle$ are the vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\ .$$

For a system of n qubits, the mathematical representation of the standard model is defined by a closed $*$-algebra (Pauli algebra) generated by the operators σ_μ^j ($\mu = x$, y, or z) that act on the j^{th} qubit:

$$\sigma_\mu^j = \overbrace{\mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes \underbrace{\sigma_\mu}_{j^{th}\text{ factor}} \otimes \cdots \otimes \mathbb{1}}^{n\text{ factors}}\ ,$$

where $\otimes$ represents a Kronecker product. The algebra satisfied by these quantum operators is

$$[\sigma_\mu^i, \sigma_\nu^j] \;\; = \;\; 2i\delta_{ij}\epsilon_{\mu\nu\lambda}\sigma_\lambda^j \; ,$$

where $[A, B] = AB - BA$, and $\epsilon_{\mu\nu\lambda}$ is the totally anti-symmetric Levi-Civita symbol.

Control of qubits is achieved by applying Hamiltonians that act on either one or two qubits. A theorem in quantum information processing says that a generic operation on a single qubit and any interaction between two qubits is sufficient for building any unitary operation. We take

$$H_P = \sum_j [\alpha_{x_j}(t) \; \sigma_x^j + \alpha_{y_j}(t) \; \sigma_y^j] + \sum_{i,j} \alpha_{ij}(t) \; \sigma_z^i \sigma_z^j, \tag{1}$$

where the $\alpha_\mu(t)$ are controllable as our control Hamiltonian for universal computation.

Similarly, we now describe a model of anyonic computation. The basic unit of this model is a state (or anyonic mode) that can be occupied by 0 or 1 anyon. We define the model through the algebra of anyon operators a_j and $a_j^\dagger$ for each qubit j $(j = 1, \cdots, n)$, i.e., through the algebra of $2n$ elements satisfying canonical equal-time commutation relations ($[A, B]_\theta = AB - e^{i\theta}BA$, with $0 \leq \theta < 2\pi$)

$$\begin{cases} [a_i, a_j]_\theta = [a_i^\dagger, a_j^\dagger]_\theta = 0 \; , \\ [a_i, a_j^\dagger]_{-\theta} = \delta_{ij}(1 - (e^{-i\theta} + 1)n_j) \; , \;\; [n_i, a_j^\dagger] = \delta_{ij} a_j^\dagger \; , \end{cases}$$

where $n_j = a_j^\dagger a_j$ and $\theta = \pi \mod(2\pi)$ corresponds to canonical fermions, while $\theta = 0 \mod(2\pi)$ represents hard-core bosons [7]. All statistical angles θ correspond to the situation where one can only put up to a single particle per single quantum state (mode) (i.e, the particles are "hard-core"). In other words, all these anyons satisfy the Pauli exclusion principle with $(a_j^\dagger)^2 = 0$.

In this case we take

$$H_P = \sum_j \left[\alpha_j(t) a_j + \tilde{\alpha}_j(t) a_j^\dagger\right] + \sum_{ij} \alpha_{ij}(t) \left(a_i^\dagger a_j + a_j^\dagger a_i\right) + \beta_{ij}(t) \; n_i n_j \; . \tag{2}$$

as the control Hamiltonian. Physical operators must be (Hermitian) products of even degree involving combinations of the creation and annihilation operators such as the terms in the last two summands of H_P.

2.2 Equivalence of Models

One could in principle use any of the two models introduced in previous Section to perform computation and, therefore, simulate a particular physical phenomenon. These were just particular examples. On the other hand, if it is possible to efficiently simulate the anyonic model by the standard model (or vice versa) then these two models of computation are equivalent. Indeed, the crux of the proof is the one-to-one mapping between the anyonic and Pauli algebras. The isomorphism is established through the generalization of the Jordan-Wigner mapping [6, 8]

$$\begin{cases} \sigma_+^j = K_j(\theta)\, a_j^\dagger \\ \sigma_-^j = a_j K_j^\dagger(\theta) \\ \sigma_z^j = 2n_j - 1 \end{cases}$$

where the statistical operator $K_j(\theta)$ is given by

$$K_j(\theta) = e^{i\theta \sum_{i<j} n_i} = \prod_{i<j} [1 + (e^{i\theta} - 1)\ n_i] \ ,$$

since $n_j^2 = n_j$ (for any $\theta \bmod(2\pi)$), and satisfy $K_j(\theta)K_j^\dagger(\theta) = K_j^\dagger(\theta)K_j(\theta) = \mathbb{1}$. The inverse mapping is:

$$\begin{cases} a_j^\dagger = \prod_{i<j} [\dfrac{e^{-i\theta}+1}{2} + \dfrac{e^{-i\theta}-1}{2}\sigma_z^i]\ \sigma_+^j \\ a_j = \prod_{i<j} [\dfrac{e^{i\theta}+1}{2} + \dfrac{e^{i\theta}-1}{2}\sigma_z^i]\ \sigma_-^j \\ n_j = \frac{1}{2}(1+\sigma_z^j) \ . \end{cases}$$

Given the polynomial scaling of the mappings (regardless of the spatial dimensionality of the lattice [5, 6]), it is always possible to efficiently map a general anyon Hamiltonian to Pauli operators which can then be simulated using the control Hamiltonians of the standard model. This establishes that these two models of computation are polynomially equivalent. So the quantum imitation using anyons is efficient if the standard model imitation is efficient (and vice versa).

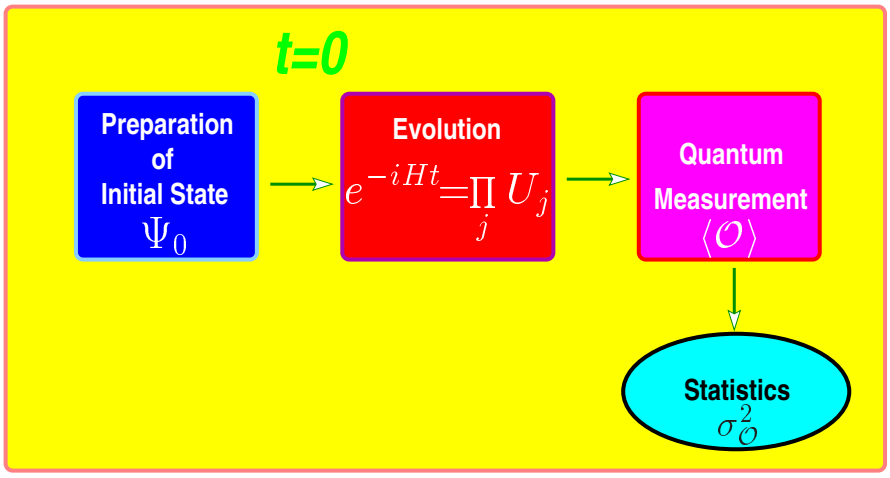

Figure 2: Schematics of a quantum algorithm: Ψ_0 is the initial state, U_j's are unitary operators, $\mathcal{O}$ is an observable and σ^2 is the variance. For an efficient imitation one needs all steps in this chain to scale polynomially with complexity.

2.3 Quantum Network Representation of Physical Phenomena

Ideally, no constraints on the control functions are assumed in Eqs. 1 and 2. However, it is often simpler to design the required control by assuming that only one of the $\alpha_\mu(t)$ is non-zero at any time (quantum gate). A quantum algorithm for this model of quantum computation consists of prescribing the control functions $\alpha_\mu(t)$ [3]. For example, for the fermionic model a universal set of quantum gates is

$$e^{i\frac{\pi}{4}(a_i^\dagger a_j + a_j^\dagger a_i)} \ , \ e^{i\frac{\pi}{4}(a_i^\dagger a_j^\dagger + a_j a_i)} \ , \ e^{i\frac{\pi}{4}n_i} \ , \ e^{i\pi n_i n_j} \ .$$

In the quantum network representation of the fermionic model, an algorithm is a specific sequence of these operators (quantum gates) applied to the initial state.

Like the simulation of a physical system on a CC, the simulation of a physical system on a QC has four basic steps (see Fig. 2): the preparation of an initial state, the unitary evolution of the initial state (the core of the algorithm), the quantum measurement of the physical properties of the evolved state, and error control. We will consider each process in turn, but first we note that on a QC there is another important consideration, namely, the relationship of the operator algebra natural to the physical

system to the algebra of the quantum network. Fortunately, the mappings (i.e., isomorphisms) between arbitrary representations of Lie algebras are now known [6] and previous Sections showed an example.

The mappings between algebras, between an algebra and a physical system, and between physical systems are necessary in order to be able to simulate physical systems using a QC fabricated on the basis of another system. However, this does not imply that the simulation of a particular physical phenomenon is efficiently implementable. As we have previously discussed [3], efficient quantum computation involves more than having the ability to represent 2^n different items of classical information so that the algebra of n qubits can be isomorphically represented and quantum parallelism can be exploited. The main focus of Ref. [3] was demonstrating that a particular problem for simulating fermions (i.e., $\theta = \pi$) on a CC, called the dynamical sign problem, does not exist on a QC. This amounts to prove the polynomial scaling of the construction of the initial state, its subsequent time propagation, measurement of some observables and control of the error in the results. Similar ideas can be followed to prove polynomial complexity in the anyonic case [9].

2.4 Resonant Impurity Scattering: An elementary example

To illustrate the concepts described above consider the simulation of a very simple physical phenomenon, using a QC with quantum spin-1/2 basic units (e.g., liquid NMR). The system to be imitated is described by the Fano-Anderson Hamiltonian

$$H = -\sum_{j=1}^{n}(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \epsilon\, d^\dagger d + \frac{\mathcal{V}}{\sqrt{n}}\sum_{j=1}^{n}(c_j^\dagger d + d^\dagger c_j)\ ,\ c_{j+n}^\dagger = c_j^\dagger\ ,$$

where c's and d represent two different types of fermionic operators with the index j labeling the lattice sites ($R_j = ja$). Suppose that the system is prepared in the initial state with $N_e \leq n$ fermions

$$|\Psi(0)\rangle = \prod_{i=0}^{N_e-1} c_{k_i}^\dagger|\mathrm{vac}\rangle\ ,\ c_{k_i}^\dagger = \frac{1}{\sqrt{n}}\sum_{j=1}^{n}\ e^{ik_iR_j}\ c_j^\dagger\ ,$$

where $k_i = \frac{2\pi m_i}{R_n}$, with m_i an integer ($-\frac{\pi}{a} < k \leq \frac{\pi}{a}$). At $t = 0^+$, a particle is injected into the impurity state d, what is the probability amplitude that the evolved state remains in the initial state ?

This choice of problem is motivated by the existence of an exact analytic solution and the fact that it reduces to a quantum network with three qubits (two qubits for the system and one qubit for measurement), therefore, being amenable to simulation in a real liquid NMR QC.

Let's show how to write a quantum algorithm to answer that question. As shown in Refs. [3] and [5] the initial state can easily be prepared with polynomial complexity. An efficient *dictionary* between algebras is realized through the mapping

$$\begin{aligned} d = \sigma_-^1 \qquad & \qquad d^\dagger = \sigma_+^1 \\ c_{k_0} = -\sigma_z^1\sigma_-^2 \qquad & \qquad c_{k_0}^\dagger = -\sigma_z^1\sigma_+^2 \\ \vdots \qquad & \qquad \vdots \\ c_{k_{n-1}} = (-1)^n\sigma_z^1\sigma_z^2\cdots\sigma_z^n\sigma_-^{n+1} \qquad & \qquad c_{k_{n-1}}^\dagger = (-1)^n\sigma_z^1\sigma_z^2\cdots\sigma_z^n\sigma_+^{n+1} \ , \end{aligned}$$

which leads to the *translated* Hamiltonian operator ($\mathcal{E}_k = -2\cos ka$)

$$2H = \left[\epsilon + \sum_{i=0}^{n-1}\mathcal{E}_{k_i}\right]\mathbb{1} + \epsilon\sigma_z^1 + \sum_{i=0}^{n-1}\mathcal{E}_{k_i}\sigma_z^{i+2} + \mathcal{V}(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2)$$

written in terms of the basic elements of the Pauli algebra (i.e., the operator language of our QC). The physical quantity to be computed is

$$G(t) = \langle\Psi(0)|d(t)d^\dagger(0)|\Psi(0)\rangle \ , \ d(t) = e^{iHt}\ d(0)\ e^{-iHt} \ ,$$

which clearly reduces the computation to a two qubits problem since

$$d(t)d^\dagger(0) = e^{i\bar{H}t}\sigma_-^1 e^{-i\bar{H}t}\sigma_+^1 \ ,$$

with

$$\bar{H} = \frac{\epsilon}{2}\sigma_z^1 - \sigma_z^2 + \frac{\mathcal{V}}{2}(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2) \ .$$

There are some symmetries in our Hamiltonian $\bar{H}$ that simplify the expression for the correlation function $G(t)$; one can easily verify that

$$G(t) = \langle e^{i\bar{H}t}\sigma_x^1 e^{-i\bar{H}t}\sigma_x^1\rangle \ .$$

A third qubit is needed for the measurement step [3, 5]: First, we prepare the system in the initial state $|\Psi(0)\rangle = |\Psi_0\rangle$ and adjoin to it one ancilla

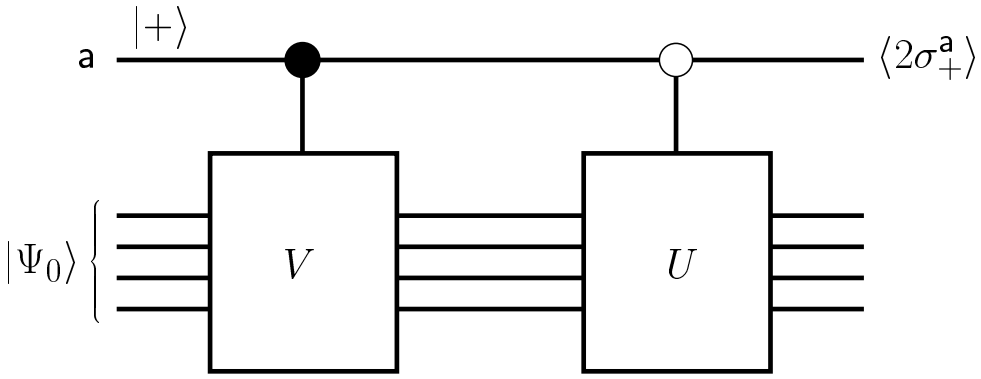

Figure 3: Measurement of the physical quantity $G(t)$ using one extra (ancilla) qubit $|\mathsf{a}\rangle$. In this case $\langle 2\sigma_+^{\mathsf{a}}\rangle = \langle\Psi_0|U^\dagger V|\Psi_0\rangle = G(t)$.

(auxiliary) qubit a, in the state $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. This is done by applying the unitary Hadamard gate to the state $|0\rangle$ [2]. Next, we make two controlled unitary evolutions using the C-V and C-U gates. The first operation $\tilde{V}$ evolves the system by $V = e^{-i\bar{H}t}\sigma_x^1$ if the ancilla is in the state $|1\rangle$: $\tilde{V} = |0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \otimes V$. The second one $\tilde{U}$ evolves the system by $U = (e^{i\bar{H}t}\sigma_x^1)^\dagger$ if the ancilla state is $|0\rangle$: $\tilde{U} = |0\rangle\langle 0| \otimes U + |1\rangle\langle 1| \otimes \mathbb{1}$. ($\tilde{V}$ and $\tilde{U}$ commute.) Once these evolutions are done, the expectation value of $2\sigma_+^{\mathsf{a}} = \sigma_x^{\mathsf{a}} + i\sigma_y^{\mathsf{a}}$ gives the desired result $\langle U^\dagger V\rangle = G(t)$. This quantum circuit is shown in Fig. 3. Note that the probabilistic nature of quantum measurements implies that the desired expectation value is obtained with variance $\mathcal{O}(1)$ for each instance. Repetition can be used to reduce the variance below what is required.

To run the simulation on a liquid NMR QC we still need to perform a decomposition of the unitary operations in terms of one qubit rotations and two qubit interactions. This is easily and exactly accomplished in this case ($2\alpha_\pm = \Delta_- \pm \sqrt{\Delta_+^2 + \mathcal{V}^2}$, $\Delta_\pm = (\epsilon \pm 2)/2$):

$$e^{-i\bar{H}t} = \mathcal{U}\, e^{-iH_{P1}t}\, \mathcal{U}^\dagger \quad \text{with} \quad H_{P1} = \alpha_-\sigma_z^1 + \alpha_+\sigma_z^2 \ \text{ and}$$

$$\mathcal{U} = e^{i\frac{\pi}{4}\sigma_x^2} e^{-i\frac{\pi}{4}\sigma_y^1} e^{-i\frac{\vartheta}{2}\sigma_z^1\sigma_z^2} e^{i\frac{\pi}{4}\sigma_y^1} e^{i\frac{\pi}{4}\sigma_x^1} e^{-i\frac{\pi}{4}\sigma_x^2} e^{-i\frac{\pi}{4}\sigma_y^2} e^{i\frac{\vartheta}{2}\sigma_z^1\sigma_z^2} e^{-i\frac{\pi}{4}\sigma_x^1} e^{i\frac{\pi}{4}\sigma_y^2} \ ,$$

where $\cos\vartheta = 1/\sqrt{1+\delta^2}$ with $\delta = (\Delta_+ + \sqrt{\Delta_+^2 + \mathcal{V}^2})/\mathcal{V}$. Figure 4 shows the result of the simulation.

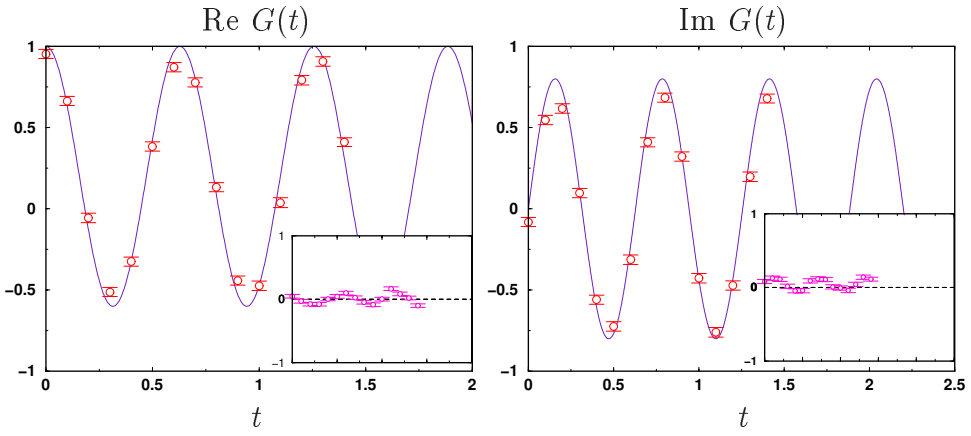

Figure 4: Real and Imaginary parts of $G(t)$ for $\epsilon = -8$, $\mathcal{V} = 4$. The continuous curves represent the exact solution while the open circles indicate the result of a simulation on a liquid NMR QC. The insets display the difference.

3 Concluding Remarks

The power of QCs over traditional computers lies in the fact that they can access and manipulate arbitrary superpositions of states, a feature known as quantum parallelism. Surprisingly, there are quantum computations, such as quantum physics simulations, with even a modest number (40) of qubits that are impossible for the biggest present day deterministic CCs. The ability to perform efficient quantum physics simulations for many degrees of freedom will bring new understanding and permit accurate prediction of the dynamics of complex quantum systems. The fact that even small numbers of qubits suffice for non-trivial computations leads to new insights into why QCs are so much more powerful.

At present, we are developing efficient algorithms for quantum physics simulations which can be implemented in present and proposed hardware for QCs, and we are studying the origin of the power of QCs. The concepts presented in this Note constitute the very first steps of a different way of thinking in simulation physics and information theory. Clearly, a number of challenges for the efficient simulation of physical systems on a quantum network remain. We are prioritizing our research on those issues associated with problems that are extremely difficult for quantum many-

body scientists to solve on CCs. Questions I would like to be answered in the next few years include: Can we find an interesting physics simulation problem that a QC can solve impossible to address with a CC? (Let's say with $\mathcal{O}(100)$ qubits). Can we efficiently simulate a continuous Quantum Field Theory with a discrete QC? Quantum Control: Is there any physical limitation to what can be really achieved?

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[7] The hard-core boson model of computation (already introduced in Ref. [3]) satisfies an algebra given by $[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$, $[b_i, b_j^\dagger] = \delta_{ij}(1 - 2n_j)$, $[n_i, b_j^\dagger] = \delta_{ij} b_j^\dagger$, and $n_j = b_j^\dagger b_j$.

[8] In the hard-core boson case (i.e., $\theta = 0 \mod(2\pi)$), the mapping is: $\sigma_+^j = b_j^\dagger$, $\sigma_-^j = b_j$, and $\sigma_z^j = 2n_j - 1$.

[9] We are aware of at least one case where the sign problem can be mapped onto a 3-SAT problem, i.e., an NP-complete problem [5]. Therefore, one cannot yet claim that a QC can solve "all" sign problems, otherwise one would claim that one is solving all NP-complete problems and this has not been rigorously established.