

Quantum computation of complex systems

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Key points

- Quantum logic: superposition and entanglement
- Quantum algorithms for complex dynamical systems
- Quantum simulations on actual quantum hardware

I. INTRODUCTION

Miniaturization provides us with an intuitive way of understanding why, in the near future, quantum mechanics will become important for computation. The electronics industry for computers grows hand-in-hand with the decrease in size of integrated circuits. This miniaturization is necessary to increase computational power, that is, the number of floating-point operations per second (flops) a computer can perform. In the 1950's, electronic computers based on vacuum-tube technology were capable of performing approximately 10^3 floating-point operations per second, while nowadays (2022) there exist supercomputers whose power is greater than 100 petaflops (a 1 petaflops computer is capable of performing 10^{15} floating-point operations per second). This enormous growth of computational power has been made possible owing to progress in miniaturization, which may be quantified empirically in Moore's law. This law is the result of a remarkable observation made by Gordon Moore in 1965: the number of transistors on a single integrated-circuit chip doubles approximately every 18 – 24 months. This exponential growth has not yet saturated and Moore's law is still valid. At the present time the limit is close to 10^{10} transistors per chip and the typical size of circuit components is of the order of 5 – 10 nanometres. Extrapolating Moore's law, it is estimated that within a few years, one would reach the atomic size for storing a single bit of information. At that point, quantum effects will become unavoidably dominant.

Quantum physics sets fundamental limitations on the size of the circuit components. The first question under debate is whether it would be more convenient to push the silicon-based transistor to its physical limits or

instead to develop alternative devices, such as quantum dots, single-electron transistors or molecular switches. A common feature of all these devices is that they are at the nanometre length scale, and therefore quantum effects play a crucial role.

So far, the quantum switches that could substitute silicon-based transistors and possibly be connected together to execute classical algorithms based on Boolean logic were discussed. In this perspective, quantum effects are simply unavoidable corrections that must be taken into account owing to the nanometre size of the switches. A quantum computer represents a radically different challenge: the aim is to build a machine based on quantum logic, that is, it processes the information and performs logic operations in agreement with the laws of quantum mechanics [1].

II. QUANTUM LOGIC

The elementary unit of quantum information is called a qubit (the quantum counterpart of the classical bit) and a quantum computer may be viewed as a many-qubit system. Physically, a qubit is a two-level system, like the two spin states of a spin-1/2 particle, the vertical and horizontal polarization states of a single photon or two levels of an atom.

A classical bit is a system that can exist in two distinct states, which are used to represent 0 and 1, that is, a single binary digit. The only possible operations (gates) in such a system are the identity ($0 \rightarrow 0, 1 \rightarrow 1$) and NOT ($0 \rightarrow 1, 1 \rightarrow 0$). In contrast, a quantum bit (qubit) is a two-level quantum system, described by a two-dimensional complex Hilbert space. In this space, one may choose a pair of normalized and mutually orthogonal quantum states, called $|0\rangle$ and $|1\rangle$ (say, the eigenstates of the Pauli operator σ_z), to represent the values 0 and 1 of a classical bit. These two states form a computational basis. From the superposition principle, any state of the qubit may be written as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad (1)$$

where the amplitudes α and β are complex numbers, constrained by the normalization condition $|\alpha|^2 + |\beta|^2 = 1$.

A quantum computer can be seen as a collection of n qubits and therefore its wave function resides in a 2^n -dimensional complex Hilbert space. While the state of an n -bit classical computer is described in binary notation

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by an integer $k \in [0, 2^n - 1]$,

$$k = k_{n-1} 2^{n-1} + \dots + k_1 2 + k_0, \quad (2)$$

with $k_0, k_1, \dots, k_{n-1} \in [0, 1]$ binary digits, the state of an n -qubit quantum computer is

$$\begin{aligned} |\psi\rangle &= \sum_{k=0}^{2^n-1} c_k |k\rangle \\ &= \sum_{k_{n-1}, \dots, k_1, k_0=0}^1 c_{k_{n-1}, \dots, k_1, k_0} |k_{n-1} \dots k_1 k_0\rangle, \quad (3) \end{aligned}$$

where $|k_{n-1} \dots k_1 k_0\rangle \equiv |k_{n-1}\rangle \otimes \dots \otimes |k_1\rangle \otimes |k_0\rangle$. Notice that the complex numbers c_k are constrained by the normalization condition $\sum_{k=0}^{2^n-1} |c_k|^2 = 1$.

The superposition principle is clearly visible in Eq. (3): while n classical bits can store only a single integer k , the n -qubit quantum register can be prepared in the corresponding state $|k\rangle$ of the computational basis, but also in a superposition. The number of states of the computational basis in this superposition can be as large as 2^n , which grows exponentially with the number of qubits. The superposition principle opens up new possibilities for computation. When one performs a computation on a classical computer, different inputs require separate runs. In contrast, a quantum computer can perform a computation for exponentially many inputs on a single run. This huge parallelism is the basis of the power of quantum computation.

The superposition principle is not a uniquely quantum feature. Indeed, classical waves satisfying the superposition principle do exist. For instance, consider the wave equation for a vibrating string with fixed endpoints. Its solutions $|\varphi_k\rangle$ satisfy the superposition principle and one can write the most general state $|\varphi\rangle$ of a vibrating string as a linear superposition of these solutions, analogously to Eq. (3): $|\varphi\rangle = \sum_{k=0}^{2^n-1} c_k |\varphi_k\rangle$. It is therefore also important to point out the importance of entanglement for the power of quantum computation, as compared to any classical computation. Entanglement is the most spectacular and counter-intuitive manifestation of quantum mechanics, observed in composite quantum systems: it signifies the existence of non-local correlations between measurements performed on well-separated particles. After two classical systems have interacted, they are in well-defined individual states. In contrast, after two quantum particles have interacted, in general, they can no longer be described independently of each other. There will be purely quantum correlations between two such particles, independently of their spatial separation. Examples of two-qubit entangled state are the four states of the so-called Bell basis, $|\phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$ and $|\psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$. The measure of the polarization state of one qubit will instantaneously affect the state of the other qubit, whatever their distance is. There is no entanglement in classical physics. Therefore, in order to represent the superposition of $N = 2^n$ levels by

means of classical waves, these levels must belong to the same system. Indeed, classical states of separate systems can never be superposed. Thus, any computation based on classical waves requires a number N of levels that grows exponentially with n . If Δ is the typical energy separation between two consecutive levels, the amount of energy required for this computation is given by $\Delta 2^n$. Hence, the amount of physical resources needed for the computation grows exponentially with n . In contrast, due to entanglement, in quantum physics a general superposition of 2^n levels may be represented by means of n qubits. Thus, the amount of physical resources (energy) grows only linearly with n .

To implement a quantum computation, one must be able to control the evolution in time of the many-qubit state describing the quantum computer. As far as the coupling to the environment may be neglected, this evolution is unitary and governed by the Schrödinger equation. It is well known that a small set of elementary logic gates allows the implementation of any complex computation on a classical computer. This is very important: it means that, when one changes the problem, one does not need to modify one's computer hardware. Fortunately, the same property remains valid for a quantum computer. It turns out that, in the quantum circuit model, any whatever complex unitary transformation acting on a many-qubit system can be decomposed into quantum gates acting on a single qubit and a suitable quantum gate acting on two qubits. Any unitary operation on a single qubit can be constructed using only Hadamard and phase-shift gates. The Hadamard gate is defined as follows: it turns $|0\rangle$ into $(|0\rangle + |1\rangle)/\sqrt{2}$ and $|1\rangle$ into $(|0\rangle - |1\rangle)/\sqrt{2}$. The phase-shift gate (of phase δ) turns $|0\rangle$ into $|0\rangle$ and $|1\rangle$ into $e^{i\delta}|1\rangle$. One can decompose a generic unitary transformation acting on a many-qubit state into a sequence of Hadamard, phase-shift and CNOT gates, where CNOT is a two-qubit gate, defined as follows: it turns $|00\rangle$ into $|00\rangle$, $|01\rangle$ into $|01\rangle$, $|10\rangle$ into $|11\rangle$, and $|11\rangle$ into $|10\rangle$. As in the classical XOR gate, the CNOT gate flips the state of the second (target) qubit if the first (control) qubit is in the state $|1\rangle$ and does nothing if the first qubit is in the state $|0\rangle$. Of course, the CNOT gate, in contrast to the classical XOR gate, can also be applied to any superposition of the computational basis states.

The decomposition of a generic unitary transformation of a n -qubit system into elementary quantum gates is in general inefficient, that is, it requires a number of gates exponentially large in n (more precisely, $O(n^2 4^n)$ quantum gates). However, there are special unitary transformations that can be computed efficiently in the quantum circuit model, namely by means of a number of elementary gates polynomial in n . A very important example is given by the quantum Fourier transform, mapping a generic n -qubit state $\sum_{k=0}^{2^n-1} a_k |k\rangle$ into $\sum_{l=0}^{2^n-1} b_l |l\rangle$, where the vector $\{b_0, \dots, b_{N-1}\}$ is the discrete Fourier transform of the vector $\{a_0, \dots, a_{N-1}\}$, that is, $b_l = \sum_{k=0}^{N-1} e^{2\pi i k l / 2^n} a_k$. It can be shown that this

transformation can be efficiently implemented in $O(n^2)$ elementary quantum gates, whereas the best known classical algorithm to simulate the Fourier transform, the fast Fourier transform, requires $O(n2^n)$ elementary operations. The quantum Fourier transform is an essential subroutine in many quantum algorithms.

III. QUANTUM ALGORITHMS

As shown above, the power of quantum computation is due to the inherent quantum parallelism associated with the superposition principle. In simple terms, a quantum computer can process a large number of classical inputs in a single run. For instance, starting from the input state $\sum_{k=0}^{2^n-1} c_k |k\rangle \otimes |0\dots 0\rangle$, one may obtain the output state

$$\sum_{k=0}^{2^n-1} c_k |k\rangle \otimes |f(k)\rangle. \quad (4)$$

Therefore, the function $f(k)$ is computed for all k in a single run (note that one needs two quantum registers to compute by means of a reversible unitary transformation $f(k)$; the second register requires enough qubits to load the output $f(k)$ for all input values $k = 0, 1, \dots, 2^n$, with n number of qubits in the first register). However, it is not an easy task to extract useful information from the output state. The problem is that this information is, in a sense, hidden. Any quantum computation ends up with a projective measurement in the computational basis: the qubit polarization is measured along the z -axis for all the qubits. The output of the measurement process is inherently probabilistic and the probabilities of the different possible outputs are set by the basic postulates of quantum mechanics. Given the state (4), one obtains $|\bar{k}\rangle|f(\bar{k})\rangle$ with probability $|c_{\bar{k}}|^2$, hence, the evaluation of the function $f(k)$ for a single $k = \bar{k}$, exactly as with a classical computer. However, there exist quantum algorithms that exploit quantum interference to efficiently extract useful information.

In 1994, Peter Shor proposed a quantum algorithm that efficiently solves the prime-factorization problem: given a composite odd positive integer N , find its prime factors. This is a central problem in computer science and it is conjectured, though not proven, that for a classical computer it is computationally difficult to find the prime factors. Indeed, the best classical algorithm, the number field sieve, requires $\exp(O(n^{1/3}(\log n)^{2/3}))$ operations. Shor's algorithm instead efficiently solves the integer factorization problem in $O((n^2 \log n \log \log n))$ elementary quantum gates, where $n = \log N$ is the number of bits necessary to code the input N . Therefore it provides an exponential improvement in speed with respect to any known classical algorithm. The integer factoring problem can be reduced to the problem of finding the period of the function $f(k) = a^k \bmod N$, where N is

the number to be factorized and $a < N$ is chosen randomly. The modular exponentiation can be computed efficiently on a quantum computer and, starting from the state $\frac{1}{\sqrt{N}} \sum_{k=0}^{2^n-1} |k\rangle|0\dots 0\rangle$ (the equal superposition of all basis states in the first register can be obtained by applying one Hadamard gate for each qubit), one arrives at $\frac{1}{\sqrt{N}} \sum_{k=0}^{2^n-1} |k\rangle|f(k)\rangle$. Notice that there are two quantum registers, the first one stores k , the second $f(k)$. By measuring the second register, one obtains the outcome $f(\bar{k})$. Thus, the quantum computer wave function collapses onto $\frac{1}{\sqrt{m}} \sum_{j=0}^{m-1} |\bar{k} + jr\rangle|f(\bar{k})\rangle$, where m is the number of k values such that $f(k) = f(\bar{k})$, and r is the period of $f(k)$, that is $f(k) = f(k+r)$. To determine the period r , one has to perform the quantum Fourier transform of the first register. The resulting wave function is peaked around integer multiples of N/r . From the measurement of this state, one can extract the period r . It is worth mentioning that there are cryptographic systems, such as RSA, that are used extensively today and that are based on the conjecture that no efficient algorithms exist for solving the prime factorization problem. Hence Shor's algorithm, if implemented on a large scale quantum computer, would break the RSA cryptosystem.

Other quantum algorithms have been developed. In particular, Grover has shown that quantum computers can also be useful for solving the problem of searching for a marked item in an unstructured database of $N = 2^n$ items. The best one can do with a classical computer is to go through the database, until one finds the solution. This requires $O(N)$ operations. In contrast, the same problem can be solved by a quantum computer in $O(\sqrt{N})$ operations. In this case, the gain with respect to classical computation is quadratic.

IV. QUANTUM SIMULATION OF PHYSICAL SYSTEMS

The simulation of quantum many-body problems on a classical computer is a difficult task as the size of the Hilbert space grows exponentially with the number of particles. For instance, if one wishes to simulate a chain of n spin-1/2 particles, the size of the Hilbert space is 2^n . Namely, the state of this system is determined by 2^n complex numbers. As observed by Feynman in the 1980's, the growth in memory requirement is only linear on a quantum computer, which is itself a many-body quantum system. For example, to simulate n spin-1/2 particles one only needs n qubits. Therefore, a quantum computer operating with only a few tens of qubits can outperform a classical computer. Of course, this is only true if one can find an efficient quantum algorithm and if one can efficiently extract useful information from the quantum computer. Quite interestingly, a quantum computer can outperform a classical computer not only for the investigation of the properties of many-body quantum systems, but also for the study of the quantum and

classical dynamics of complex single-particle systems.

For a concrete example, consider the quantum-mechanical motion of a particle in one dimension (the extension to higher dimensions is straightforward). It is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} \psi(x, t) = H \psi(x, t), \quad (5)$$

where the Hamiltonian H is given by

$$H = H_0 + V(x, t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x, t). \quad (6)$$

The Hamiltonian $H_0 = -(\hbar^2/2m) d^2/dx^2$ governs the free motion of the particle, while $V(x, t)$ is a (possibly time-dependent) one-dimensional potential. To solve Eq. (5) on a quantum computer with finite resources (a finite number of qubits and a finite sequence of quantum gates), one must first of all discretize the continuous variables x and t . If the motion essentially takes place inside a finite region, say $-d \leq x \leq d$, decompose this region into 2^n intervals of length $\Delta = 2d/2^n$ and represent these intervals by means of the Hilbert space of an n -qubit quantum register (this means that the discretization step drops exponentially with the number of qubits). Hence, the wave function $|\psi(t)\rangle$ is approximated as follows:

$$|\tilde{\psi}(t)\rangle = \frac{1}{\mathcal{N}} \sum_{i=0}^{2^n-1} \psi(x_i, t) |i\rangle, \quad (7)$$

where $x_i \equiv -d + (i + \frac{1}{2}) \Delta$, $|i\rangle = |i_{n-1}\rangle \otimes \cdots \otimes |i_0\rangle$ is a state of the computational basis of the n -qubit quantum register and $\mathcal{N} \equiv \sqrt{\sum_{i=0}^{2^n-1} |\psi(x_i, t)|^2}$ is a factor that ensures correct normalization of the wave function. It is intuitive that $|\tilde{\psi}\rangle$ provides a good approximation to $|\psi\rangle$ when the discretization step Δ is much smaller than the shortest length scale relevant for the motion of the system. The Schrödinger equation (5) may be integrated by propagating the initial wave function $\psi(x, 0)$ for each time-step ϵ as follows:

$$\psi(x, t + \epsilon) = e^{-\frac{i}{\hbar}[H_0+V(x,t)]\epsilon} \psi(x, t). \quad (8)$$

If the time-step ϵ is small enough, it is possible to write the Trotter decomposition

$$e^{-\frac{i}{\hbar}[H_0+V(x,t)]\epsilon} \approx e^{-\frac{i}{\hbar}H_0\epsilon} e^{-\frac{i}{\hbar}V(x,t)\epsilon}, \quad (9)$$

which is exact up to terms of order ϵ^2 . The operator on the right-hand side of Eq. (9) is still unitary, simpler than that on the left-hand side, and, in many interesting physical problems, can be efficiently implemented on a quantum computer. Advantage is taken of the fact that the Fourier transform can be efficiently performed by a quantum computer. One can then write the first operator in the right-hand side of (9) as

$$e^{-\frac{i}{\hbar}H_0\epsilon} = F^{-1} e^{+\frac{i}{\hbar}\left(\frac{\hbar^2 k^2}{2m}\right)\epsilon} F, \quad (10)$$

where k is the variable conjugated to x and F the discrete Fourier transform. This represents a transformation from the x -representation to the k -representation, in which this operator is diagonal. Then, using the inverse Fourier transform F^{-1} , one returns to the x -representation, in which the operator $\exp(-iV(x, t)\epsilon/\hbar)$ is diagonal. The wave function $\psi(x, t)$ at time $t = l\epsilon$ is obtained from the initial wave function $\psi(x, 0)$ by applying l times the unitary operator

$$F^{-1} e^{+\frac{i}{\hbar}\left(\frac{\hbar^2 k^2}{2m}\right)\epsilon} F e^{-\frac{i}{\hbar}V(x,t)\epsilon}. \quad (11)$$

Therefore, simulation of the Schrödinger equation is now reduced to the implementation of the Fourier transform plus diagonal operators of the form

$$|x\rangle \rightarrow e^{icf(x)} |x\rangle, \quad (12)$$

where c is some real constant. Note that an operator of the form (12) appears both in the computation of $\exp(-iV(x, t)\epsilon/\hbar)$ and of $\exp(-iH_0\epsilon/\hbar)$, when this latter operator is written in the k -representation. The quantum computation of (12) is possible, using an ancillary quantum register $|y\rangle_a$, by means of the following steps:

$$\begin{aligned} |0\rangle_a \otimes |x\rangle &\rightarrow |f(x)\rangle_a \otimes |x\rangle \rightarrow e^{icf(x)} |f(x)\rangle_a \otimes |x\rangle \\ &\rightarrow e^{icf(x)} |0\rangle_a \otimes |x\rangle = |0\rangle_a \otimes e^{icf(x)} |x\rangle. \end{aligned} \quad (13)$$

The first step is a standard function evaluation and may be implemented by means of $O(n2^n)$ elementary quantum gates. Of course, more efficient implementations (polynomial in n) are possible when the function $f(x)$ has some structure, as it is the case for the potentials $V(x, t)$ usually considered in quantum-mechanical problems. The second step in (13) is the transformation $|y\rangle_a \rightarrow e^{icy}|y\rangle_a$ and can be performed in m single-qubit phase-shift gates, m being the number of qubits in the ancillary register. Indeed, one may write the binary decomposition of an integer $y \in [0, 2^m - 1]$ as $y = \sum_{j=0}^{m-1} y_j 2^j$, with $y_j \in \{0, 1\}$. Therefore,

$$\exp(iy) = \exp\left(\sum_{j=0}^{m-1} icy_j 2^j\right) = \prod_{j=0}^{m-1} \exp(icy_j 2^j), \quad (14)$$

which is the product of m single-qubit gates, each acting non-trivially (differently from identity) only on a single qubit. The j -th gate operates the transformation $|y_j\rangle_a \rightarrow \exp(icy_j 2^j)|y_j\rangle_a$, with $|y_j\rangle_a \in \{|0\rangle, |1\rangle\}$ vectors of the computational basis for the j -th ancillary qubit. The third step in (13) is just the reverse of the first and may be implemented by the same array of gates as the first but applied in the reverse order. After this step the ancillary qubits are returned to their standard configuration $|0\rangle_a$ and it is therefore possible to use the same ancillary qubits for every time-step. Note that the number of ancillary qubits m determines the resolution in the computation of the diagonal operator (12). Indeed, the function $f(x)$ appearing in (12) is discretized and can take 2^m different values.

An example of an interesting dynamical model that can be simulated efficiently (and without ancillary qubits) on a quantum computer is the so-called quantum sawtooth map. This map represents the dynamics of a periodically driven system and is derived from the Hamiltonian

$$H(\theta, I; \tau) = \frac{I^2}{2} + V(\theta) \sum_{j=-\infty}^{+\infty} \delta(\tau - jT), \quad (15)$$

where (I, θ) are conjugate action-angle variables ($0 \leq \theta < 2\pi$), with the usual quantization rules, $\theta \rightarrow \theta$ and $I \rightarrow I - i\partial/\partial\theta$ (set $\hbar = 1$) and $V(\theta) = -k(\theta - \pi)^2/2$. This Hamiltonian is the sum of two terms, $H(\theta, I; \tau) = H_0(I) + U(\theta; \tau)$, where $H_0(I) = I^2/2$ is just the kinetic energy of a free rotator (a particle moving on a circle parametrized by the coordinate θ), while $U(\theta; \tau) = V(\theta) \sum_j \delta(\tau - jT)$ represents a force acting on the particle that is switched on and off instantaneously at time intervals T . Therefore, it is said that the dynamics described by Hamiltonian (15) is kicked. The (quantum) evolution from time tT^- (prior to the t -th kick) to time $(t+1)T^-$ (prior to the $(t+1)$ -th kick) is described by a unitary operator U acting on the wave function ψ :

$$\begin{aligned} \psi_{t+1} &= U \psi_t = U_T U_k \psi_t; \\ U_T &= e^{-iT^2/2}, \quad U_k = e^{ik(\theta-\pi)^2/2}. \end{aligned} \quad (16)$$

This map is called the quantum sawtooth map, since the force $F(\theta) = -dV(\theta)/d\theta = k(\theta - \pi)$ has a sawtooth shape, with a discontinuity at $\theta = 0$.

In the following, an exponentially efficient quantum algorithm for simulation of the map (16) is described. It is based on the forward/backward quantum Fourier transform between action and angle bases. Such an approach is convenient since the operator U is the product of the two operators U_k and U_T , which are diagonal in the θ and I representations, respectively. This quantum algorithm requires the following steps for one map iteration:

1. Apply U_k to the wave function $\psi(\theta)$. In order to decompose the operator U_k into one- and two-qubit gates, we first of all write θ in binary notation:

$$\theta = 2\pi \sum_{j=1}^n \alpha_j 2^{-j}, \quad (17)$$

with $\alpha_i \in \{0, 1\}$. Here n is the number of qubits, so that the total number of levels in the quantum sawtooth map is $N = 2^n$. One can insert (17) into the unitary operator U_k , obtaining the decomposition

$$e^{ik(\theta-\pi)^2/2} = \prod_{i,j=1}^n e^{i2\pi^2 k(\alpha_i 2^{-i} - \frac{1}{2^n})(\alpha_j 2^{-j} - \frac{1}{2^n})}, \quad (18)$$

which is the product of n^2 two-qubit gates, each acting non-trivially only on the 4-dimensional subspace spanned by the qubits i and j .

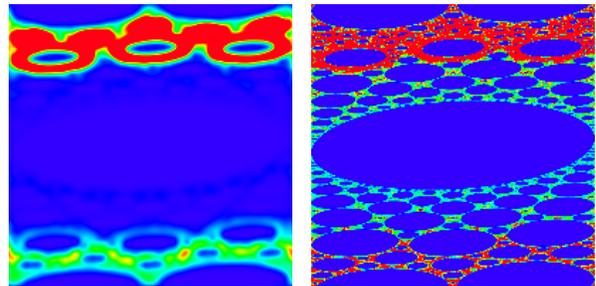


FIG. 1: Husimi function for the sawtooth map for $n = 9$ (left) and $n = 16$ (right) qubits, in action angle variables (I, θ) , with $-N/2 \leq I < N/2$ (vertical axis, $N = 2^n$) and $0 \leq \theta < 2\pi$ (horizontal axis), averaged in the interval $950 \leq t \leq 1000$, for $T = 2\pi/N$ and $kT = -0.1$. An action eigenstate, $|\psi_0\rangle = |m_0\rangle$, with $m_0 = [0.38N]$ is considered as initial state at time $t = 0$. The color is proportional to the density: blue for zero and red for maximal density.

2. The change from the θ to the I representation is obtained by means of the quantum Fourier transform, which requires $\frac{1}{2}n(n+1)$ elementary quantum gates.
3. In the I representation, the operator U_T has essentially the same form as the operator U_k in the θ representation, and therefore it can be decomposed into n^2 two-qubit gates, similarly to Eq. (18).
4. Return to the initial θ representation by application of the inverse quantum Fourier transform.

Thus, overall, this quantum algorithm requires $3n^2 + n$ gates per map iteration. This number is to be compared with the $O(n2^n)$ operations required by a classical computer to simulate one map iteration by means of a fast Fourier transform. Thus, the quantum simulation of the quantum sawtooth map dynamics is exponentially faster than any known classical algorithm. Note that the resources required to the quantum computer to simulate the evolution of the sawtooth map are only logarithmic in the Hilbert space dimension N .

As an example of the efficiency of this quantum algorithm, Fig. 1 shows the Husimi functions, taken after 1000 map iterations. It is noted that $n = 9$ qubits are sufficient to observe the appearance of integrable islands, while at $n = 16$ these islands exhibit a complex hierarchical structure in the phase space.

However, there is an additional aspect to be taken into account. Any quantum algorithm has to address the problem of efficiently extracting useful information from the quantum computer wave function. Indeed, the result of the simulation of a quantum system is the wave function of this system, encoded in the n qubits of the quantum computer. The problem is that, in order to measure all $N = 2^n$ wave function coefficients by means of standard polarization measurements of the n qubits, one has to repeat the quantum simulation a number of times exponential in the number of qubits. This procedure would

spoil any quantum algorithm, even in the case, like the present one, in which such algorithm could compute the wave function with an exponential gain with respect to any classical computation. Nevertheless, there are some important physical questions that can be answered in an efficient way.

The quantum computation can provide an exponential gain (with respect to any known classical computation) in problems that require the simulation of dynamics up to a time t which is independent of the number of qubits. In this case, provided that one can extract the relevant information in a number of measurements polynomial in the number of qubits, one should compare, in the example of the quantum sawtooth map, $O(t(\log N)^2)$ elementary gates (quantum computation) with $O(tN \log N)$ elementary gates (classical computation). This is, for instance, the case of dynamical correlation functions of the form

$$C_t \equiv \langle \psi_0 | A_t^\dagger B_0 | \psi_0 \rangle = \langle \psi_0 | (U^\dagger)^t A_0^\dagger U^t B_0 | \psi_0 \rangle, \quad (19)$$

where U is the time-evolution operator (16) for the quantum sawtooth map. Similarly, one can efficiently compute the fidelity of quantum motion, which is a quantity of central interest in the study of the stability of quantum motion under perturbations. The fidelity $f(t)$ (also called the Loschmidt echo), measures the accuracy with which a quantum state can be recovered by inverting, at time t , the dynamics with a perturbed Hamiltonian. It is defined as

$$f(t) = \langle \psi | (U_\epsilon^\dagger)^t U^t | \psi \rangle = \langle \psi | e^{iH_\epsilon t} e^{-iHt} | \psi \rangle. \quad (20)$$

Here the wave vector $|\psi\rangle$ evolves forward in time with Hamiltonian H up to time t and then evolves backward in time with a perturbed Hamiltonian H_ϵ . If the evolution operators U and U_ϵ can be simulated efficiently on a quantum computer, as is the case in many physically interesting situations, then the fidelity of quantum motion can be evaluated with exponential speed up with respect to known classical computations. As shown in Fig. 2, it is possible to measure the fidelity by means of a Ramsey-type quantum interferometer method. A single ancillary qubit is needed, initially prepared in the state $|0\rangle$, while the input state for the other n qubits is a given initial state $|\psi_0\rangle$ for the quantum sawtooth map. Two Hadamard gates are applied to the ancillary qubit, and in between these operations a controlled- W operation is applied (W is a unitary operator), namely W is applied to the other n qubits only if the ancillary qubit is in its $|1\rangle$ state. As a result, one obtains the following final overall state for the $n+1$ qubits:

$$\frac{1}{2} [(|0\rangle + |1\rangle)|\psi_0\rangle + (|0\rangle - |1\rangle)W|\psi_0\rangle]. \quad (21)$$

If $W = (U_\epsilon^\dagger)^t U^t$, then one can derive the fidelity from polarization measurements of the ancillary qubit. One obtains

$$f(t) = \langle \sigma_z \rangle^2 + \langle \sigma_y \rangle^2, \quad (22)$$

where $\langle \sigma_z \rangle$ and $\langle \sigma_y \rangle$ are the expectation values of the Pauli operators σ_z and σ_y . Provided that the quantum algorithm implementing U is efficient, as it is the case for the quantum sawtooth map, the fidelity can then be computed efficiently.

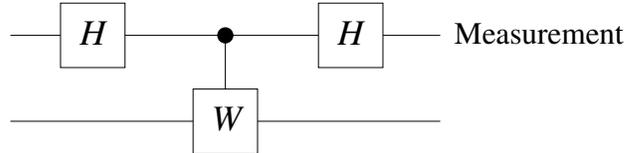


FIG. 2: Schematic drawing of a quantum circuit implementing a Ramsey-type quantum interferometer. The top line denotes a single ancillary qubit, the bottom line a set of n qubits, H the Hadamard gate and W a unitary transformation.

V. SIMULATING COMPLEX DYNAMICS ON ACTUAL QUANTUM HARDWARE

Present-day quantum computers, whether they are based on superconducting qubits or on trapped ions, suffer from significant decoherence and the effects of various noise sources. Therefore, achieving the quantum advantage in practically relevant problems such as chemical reactions, new materials design, or biological processes, is an imposing task. Note that quantum advantage is achieved when a quantum computer can solve a problem that no classical computer can solve in a feasible amount of time. The progress of currently available quantum processors can nevertheless be benchmarked by simulating complex dynamics.

An illustrative example is again provided by the quantum sawtooth map. The classical limit of such map is chaotic when $kT < -4$ or $kT > 0$. Although the sawtooth map is a deterministic system, in the chaotic regime the motion along the action direction is in practice indistinguishable from a random walk, with diffusion in the action variable. If one considers a classical ensemble of trajectories with fixed initial action m_0 and random initial angle θ , the second moment of the action distribution grows linearly with the number t of map iterations, $\langle (\Delta I)^2 \rangle \approx D(k)t$, with a diffusion coefficient D dependent on k . The quantum sawtooth map, in agreement with the correspondence principle, initially exhibits diffusive behavior, with the classical diffusion coefficient D . However, after a break time t^* , quantum interference leads to suppression of diffusion. For $t > t^*$, the quantum distribution reaches a steady state which decays exponentially over the action eigenbasis:

$$W_m \equiv |\langle m | \psi \rangle|^2 \approx \frac{1}{\ell} \exp\left[-\frac{2|m - m_0|}{\ell}\right], \quad (23)$$

where the index m singles out the action eigenstates ($I|m\rangle = m|m\rangle$), the system is initially prepared in the

eigenstate $|m_0\rangle$, and ℓ is known as the localization length of the system. Therefore, for $t > t^*$ only

$$\sqrt{\langle(\Delta I)^2\rangle} \approx \sqrt{Dt^*} \approx \ell \quad (24)$$

levels are populated. This phenomenon, known as dynamical localization, is due to quantum interference effects, suppressing the underlying classical diffusion process after a time $t^* \approx \ell \approx D$.

Fig. 3 shows the results of a dynamical localization experiment with $n = 3$ qubits on a real and freely available IBM quantum processor, with superconducting qubits, remotely accessed through cloud quantum programming [2]. The initial condition is peaked in action, $\psi_0(m) = \langle m|\psi_0\rangle = \delta_{m,m_0}$, with $m_0 = 0$. The quantum algorithm for the sawtooth map allows one to compute the wave vector $\psi_t(m)$ as a function of the number of map steps, and then the probability distribution $W_t(m) = |\psi_t(m)|^2$. In the figure $k \approx 0.273 < 1$, so that the distribution is already localized after a single map step. On the other hand, here $kT = 1.5$, corresponding to diffusive, chaotic behavior for the underlying classical dynamics. In Fig. 3 the ideal, noiseless distribution after $t = 1$ map step is compared with the results of the real quantum hardware and with a simulator (Qiskit, provided by IBM), which takes into account a few relevant noise sources, modeling in particular dephasing, relaxation, and readout errors. The results show that the quantum hardware exhibits a localization peak, which emerges from quantum interference. Note that the quantum algorithm performs forward-backward Fourier transform, thus exploring the entire Hilbert space of the quantum register in a complex multiple-path interferometer that leads to wave-function localization. As such, dynamical localization is a very fragile quantum phenomenon, extremely sensitive to noise. The height of the peak, is significantly smaller than the noiseless value and the prediction of the Qiskit simulator. These results show that the Qiskit simulator underestimate some of the relevant noise channels, such as fluctuations of the qubit quality parameters between calibrations of the quantum computer, memory effects, and cross-talks between qubits.

The presence of these noise channels also shows the imposing difficulties in scaling quantum algorithms to a large number of qubits and of quantum gates. On the other hand, striking progress has been reported in recent years, quantified for instance by the quantum volume V_Q , a single number meant to encapsulate the quantum computer performance, including number of available qubits and number of quantum gates that can be reliably implemented, before errors dominate [3]. The quantum volume is defined as

$$\log_2 V_Q = \arg \max_{\kappa \leq n} \{\min[\kappa, d(\kappa)]\}, \quad (25)$$

where n is the number of qubits in the quantum computer, and $d(\kappa) = 1/(\kappa \epsilon_{\text{eff}}(\kappa))$, known as circuit depth, is determined by an effective error rate $\epsilon_{\text{eff}}(\kappa)$ for a subset of $\kappa \leq n$ qubits, on which sequences of random two-qubit

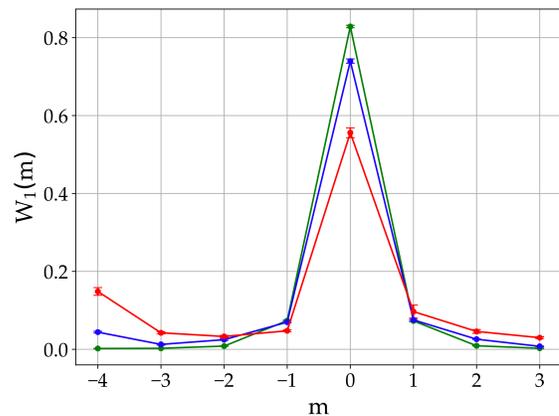


FIG. 3: Dynamical localization in the quantum sawtooth map with $n = 3$ qubits, $kT = 1.5$, $k \approx 0.273$. Data from the IBM quantum processors *lima* (red) are obtained after averaging over 10 repetitions of 8192 experimental runs, and compared with the Qiskit simulator (blue) and the noiseless simulation (green).

unitaries are implemented. From January, 2020 to December, 2021, the reported values of V_Q have increased from $V_Q = 32$ to $V_Q = 2048$ (for a comparison, data from Fig. 3 have been obtained with a machine with quantum volume $V_Q = 8$).

VI. OUTLOOK

A few significant examples have been discussed showing the capabilities of a quantum computer in the simulation of complex physical systems. A quantum computer with a few tens of qubits and a long enough decoherence time to allow the implementation of a large number of quantum gates, would outperform a classical computer in this kind of problems.

Any practical implementation of a quantum computer has to face errors, due to the inevitable coupling of the computer to the surrounding environment or to imperfections in the quantum computer hardware. The first kind of error is known as decoherence and is a threat to the actual implementation of any quantum computation. More generally, decoherence theory has a fundamental interest beyond quantum information science, since it provides explanations for the emergence of classicality in a world governed by the laws of quantum mechanics [4]. The core of the problem is the superposition principle, according to which any superposition of quantum states is an acceptable quantum state. This entails consequences that are absurd according to classical intuition, like the superposition of “cat alive” and “cat dead” that is considered in the Schrödinger’s cat paradox. The interaction with the environment can destroy the coherence between the states appearing in a superposition (for instance, the “cat alive” and “cat dead” states). Therefore, decoherence invalidates the quantum superposition principle, which is

at the heart of the power of quantum algorithms. The presence of device imperfections, although not leading to any decoherence, also hinders the implementation of any quantum computational task, introducing errors. Therefore, decoherence and imperfection effects appear to be the ultimate obstacle to the realization of a large-scale quantum computer.

Note that a quantum computer is not necessarily required for implementing quantum simulation. Simpler quantum devices, called (analog) quantum simulators can mimic the evolution of other quantum systems in an analog manner. Such simulators are problem-specific quantum machines, namely controllable quantum systems used to simulate other quantum systems [5].

At present (2022) it is not clear if and when a useful quantum computer, capable of outperforming existing classical computers in important computational tasks, will be built. In order to perform coherent controlled

evolution of a many-qubit system, one needs to take into account the problem of decoherence, and therefore large-scale quantum computers appear unrealistic with present technology. On the other hand, progress in the field has been huge in recent years. Moreover, we should bear in mind that technological breakthroughs (such as the transistor was for the classical computer) are always possible and that no fundamental objections have been found against the possibility of building a quantum computer.

Acknowledgments

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- [1] G. Benenti, G. Casati, D. Rossini, and G. Strini, *Principles of Quantum Computation and Information* (A comprehensive textbook) (World Scientific, Singapore, 2019).
 - [2] A. Pizzamiglio, S. Y. Chang, M. Bondani, S. Montangero, D. Gerace, and G. Benenti, *Dynamical localization simulated on actual quantum hardware*, *Entropy* **23**, 654 (2021).
 - [3] A. W. Cross, L. S. Bishop, S. Sheldon, P. D. Nation, and J. M. Gambetta, *Validating quantum computers using randomized model circuits*, *Phys. Rev. A* **100**, 032328 (2019).
 - [4] W.H. Zurek, *Decoherence, einselection, and the quantum origins of the classical*, *Rev. Mod. Phys.* **75**, 715 (2003).
 - [5] I. M. Georgescu, A. Ashhab, and F. Nori, *Quantum simulation*, *Rev. Mod. Phys.* **86**, 153 (2014).

VII. KEYWORDS

quantum computers
 quantum algorithms
 quantum simulation
 quantum logic
 superposition principle
 entanglement
 quantum measurements
 information extraction
 dynamical systems