Quantum simulation of the single-particle Schrödinger equation

Giuliano Benenti\textsuperscript{1,2,*} and Giuliano Strini\textsuperscript{3,†}

\textsuperscript{1}CNISM, CNR-INFM \& Center for Nonlinear and Complex Systems, Università degli Studi dell’Insubria, Via Valleggio 11, 22100 Como, Italy
\textsuperscript{2}Istituto Nazionale di Fisica Nucleare, Sezione di Milano, via Celoria 16, 20133 Milano, Italy
\textsuperscript{3}Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

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The working of a quantum computer is described in the concrete example of a quantum simulator of the single-particle Schrödinger equation. We show that a register of 6 – 10 qubits is sufficient to realize a useful quantum simulator capable of solving in an efficient way standard quantum mechanical problems.

I. INTRODUCTION

During the last years quantum information\textsuperscript{1,2} has become one of the new hot topic field in physics, with the potential to revolutionize many areas of science and technology. Quantum information replaces the laws of classical physics, applied to computation and communication, with the more fundamental laws of quantum mechanics. This becomes increasingly important due to technological progress reaching smaller and smaller scales. Extrapolating the miniaturization process of integrated circuits one would estimate that we shall reach the atomic size for storing a single bit of information around the year 2020 (at the present time the typical size of circuit components is of the order of 100 nanometers). At that point, quantum effects will become unavoidably dominant.

The final aim of quantum computation is to build a machine based on quantum logic, that is, a machine that can process the information and perform logic operations in agreement with the laws of quantum mechanics. In addition to its fundamental interest, a large scale quantum computer, if constructed, would advance computing power beyond the capabilities of classical computation.

The purpose of the present paper is to illustrate the main features of a quantum computer in the concrete example of a quantum simulator of the single-particle Schrödinger equation. We wish to show that quantum logic, already with a small number of qubits, allows the efficient simulation of basic quantum mechanical problems. A quantum simulator with 6 – 10 qubits could produce a real picture book of quantum mechanics. We believe that snapshots from this book will help develop a physical intuition of the power of quantum computation.

Our paper adds to other existing pedagogical presentations of various aspects of quantum computation, including Shor’s quantum algorithm for integer factorization\textsuperscript{4}, Grover’s quantum search algorithm\textsuperscript{5,6}, quantum information processing by means of nuclear magnetic resonance techniques\textsuperscript{7}, using linear optics\textsuperscript{9}, with cold atoms and ions\textsuperscript{8}, or with superconducting circuits\textsuperscript{9}, quantum measurements\textsuperscript{10}, decoherence\textsuperscript{11}, quantum error-correction and fault-tolerant quantum computation\textsuperscript{12}.

II. QUANTUM LOGIC

The elementary unit of quantum information is the 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-\(\frac{1}{2}\) particle, the polarization states of a single photon or two states 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 (classical gates) in such a system are the identity (0 → 0, 1 → 1) and NOT (0 → 1, 1 → 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, 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

\begin{equation}
|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,
\end{equation}

where the amplitudes \(\alpha\) and \(\beta\) are complex numbers, constrained by the normalization condition \(|\alpha|^2 + |\beta|^2 = 1\). Moreover, state vectors are defined up to a global phase of no physical significance. Therefore, \(|\psi\rangle\) only depends on two real parameters and we may write \(|\psi\rangle = \cos \frac{\theta}{2}|0\rangle + e^{i\phi}\sin \frac{\theta}{2}|1\rangle\), with \(0 \leq \theta \leq \pi\) and \(0 \leq \phi < 2\pi\).

A collection of \(n\) qubits is known as a quantum register of size \(n\). 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 by an integer \(k \in \{0, 1, ..., 2^n - 1\}\),

\begin{equation}
k = k_{n-1}2^{n-1} + \cdots + k_12 + k_0,
\end{equation}

with \(k_0, k_1, \ldots, k_{n-1} \in \{0, 1\}\) binary digits, the state of an \(n\)-qubit quantum computer is

\begin{equation}
|\psi\rangle = \sum_{k=0}^{2^n-1} c_k|k\rangle,
\end{equation}

where \(|k\rangle \equiv |k_{n-1}\rangle \cdots |k_1\rangle |k_0\rangle\), with \(|k_j\rangle\) state of the \(j\)-th qubit, and \(\sum_{k=0}^{2^n-1} |c_k|^2 = 1\). Note that we use the shorthand notation \(|k_{n-1}\rangle \cdots |k_1\rangle |k_0\rangle\) for the tensor product.
Taking into account the normalization condition and the fact that a quantum state is only defined up to an overall phase, the state of an $n$-qubit quantum computer is determined by $2 \times 2^n - 2$ independent real parameters.

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. We stress that 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 efficient computation. When we perform 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.

We stress that the superposition principle is not a uniquely quantum feature. Indeed, classical waves satisfying the superposition principle do exist. For instance, we may consider the wave equation for a vibrating string 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 $\delta$) turns $|0\rangle$ into $|0\rangle$ and $|1\rangle$ into $e^{i\delta}|1\rangle$. Since global phases have no physical meaning, the states of the computational basis, $|0\rangle$ and $|1\rangle$, are unchanged. However, a generic single-qubit state $\alpha|0\rangle + \beta|1\rangle$ is mapped into $\alpha|0\rangle + \beta e^{i\delta}|1\rangle$. Since relative phases are observable, the state of the qubit has been changed by the application of the phase-shift gate. We can decompose a generic unitary transformation acting on a many-qubit system into a sequence of Hadamard, phase-shift and controlled-not (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 an $n$-qubit system into elementary quantum gates is in general inefficient, that is, it requires a number of gates exponentially large in $n$ (more precisely, $O(n^2 2^n)$ quantum gates). However, there are unitary transformations that can be computed efficiently in the quantum circuit model, namely by means of a number of elementary gates polynomial in $n$. This is the case in many computational problems of interest. A very important example is given by the quantum Fourier transform, mapping a generic $n$-qubit state $\sum_{k=0}^{2^n-1} f(k)|k\rangle$ into $\sum_{l=0}^{2^n-1} f(l)|l\rangle$, where $N = 2^n$ and the vector $\{f(0),...,f(N-1)\}$ is the discrete Fourier transform of the vector $\{f(0),...,f(N-1)\}$, that is, $f(l) = \frac{1}{\sqrt{N}} \sum_{k=0}^{2^n-1} e^{2\pi i kl/N} f(k)$. It can be shown that this transformation can be efficiently implemented in $O(n^2 = (\log_2 N)^2)$ elementary quantum gates, whereas the best known classical algorithm to simulate the Fourier transform, the fast Fourier transform,
requires $O(N \log_2 N)$ elementary operations. A quantum circuit computing the quantum Fourier transform is shown in Fig. 1: it requires $n$ Hadamard and $n(n-1)/2$ controlled phase-shift gates. By definition, the controlled phase-shift gate $C\text{PHASE}(\frac{2\pi}{p})$ we draw a circle on the control qubit and a square with $R_k$ written inside on the target qubit. Note that to implement the inverse Fourier transform it is sufficient to run the circuit in this figure from right to left and with $R_k^\dagger$ instead of $R_k$. This is due to the facts that the Hadamard gate is self-inverse and $R_k^\dagger = R_k^{-1}$.

III. QUANTUM ALGORITHMS

As we have seen, 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 $\sum_{k=0}^{2^n-1} c_k|k\rangle|0\rangle$, we may obtain the output state

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

(4)

Therefore, we have computed the function $f(k)$ for all $k$ in a single run. Note that a quantum computer implements reversible unitary transformations and that we need two quantum registers in (4) to compute in a reversible way a generic function $f$. We emphasize that 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: we measure the qubit polarization (0 or 1) 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), we obtain outcome $|k\rangle|f(k)\rangle$ with probability $|c_k|^2$. Hence, we end up with the evaluation of the function $f(k)$ for a single $k = k$, exactly as with a classical computer. Nevertheless, there exist quantum algorithms that exploit quantum interference to efficiently extract useful information. Note that in principle one could consider more general, non projective measurements. However, this would not modify considerations on the efficiency of a given quantum algorithm. The reason is that generalized measurements, after the addition of ancillary qubits, can always be represented by unitary transformations followed by standard projective measurements.

In 1994, Shor discovered a quantum algorithm which factorizes large integers exponentially faster than any known classical algorithm. It was also shown by Grover that the search of an item in an unstructured database can be done with a square root speed up over any classical algorithm. A third relevant class of quantum algorithms is the simulation of physical systems. In particular, the power of a quantum computer is intuitive for quantum many-body problems. It is indeed well known that the simulation of such 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 we wish to simulate a chain of $n$ spin-$\frac{1}{2}$ 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-$\frac{1}{2}$ particles we only need $n$ 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 we can find efficient quantum algorithms to extract useful information from the quantum computer. Quite interestingly, it has been shown that a quantum computer can be useful 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. As we shall see in the next section, basic quantum mechanical problems already can be simulated with $6-10$ qubits, while about $40$ qubits would allow one to make computations inaccessible to today’s supercomputers. We note that this figure has to be compared with the more than $1000$ qubits required to the Shor’s algorithm to outperform classical computations. Moreover, these estimates neglect the computational overhead needed to correct errors and error-correction becomes necessary to obtain reliable results by means of a large-scale quantum computer.

FIG. 1: A quantum circuit implementing the quantum Fourier transform (except for the fact that the order of qubits in the output is reversed, so that one has simply to relabel qubits in the output state). As usual in the graphical representation of quantum circuits, each line corresponds to a qubit and any sequence of logic gates must be read from the left (input) to the right (output). From bottom to top, qubits run from the least significant ($k_0$, according to binary notation (2)) to the most significant ($k_{n-1}$). Here a qubit is said to be more significant than another if its flip gives a larger variation in the integer number coded by the state of the $n$ qubits. A square with $H$ written inside stands for the Hadamard gate, while for controlled-phase shift gates $C\text{PHASE}(\frac{2\pi}{p})$ gates we draw a circle on the control qubit and a square with $R_k$ written inside on the target qubit. Note that to implement the inverse Fourier transform it is sufficient to run the circuit in this figure from right to left and with $R_k^\dagger$ instead of $R_k$. This is due to the facts that the Hadamard gate is self-inverse and $R_k^\dagger = R_k^{-1}$. 

As we have seen, 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 $\sum_{k=0}^{2^n-1} c_k|k\rangle|0\rangle$, we may obtain the output state $\sum_{k=0}^{2^n-1} c_k|k\rangle|f(k)\rangle$. Therefore, we have computed the function $f(k)$ for all $k$ in a single run. Note that a quantum computer implements reversible unitary transformations and that we need two quantum registers in (4) to compute in a reversible way a generic function $f$. We emphasize that 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: we measure the qubit polarization (0 or 1) 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), we obtain outcome $|k\rangle|f(k)\rangle$ with probability $|c_k|^2$. Hence, we end up with the evaluation of the function $f(k)$ for a single $k = k$, exactly as with a classical computer. Nevertheless, there exist quantum algorithms that exploit quantum interference to efficiently extract useful information. Note that in principle one could consider more general, non projective measurements. However, this would not modify considerations on the efficiency of a given quantum algorithm. The reason is that generalized measurements, after the addition of ancillary qubits, can always be represented by unitary transformations followed by standard projective measurements.

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IV. THE QUANTUM SIMULATOR

To illustrate the working of a quantum algorithm by means of a concrete example, let us consider the quantum-mechanical motion of a particle in one dimension (the extension to higher dimensions is straightforward)\textsuperscript{13,14,15}. 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
\[ H = H_0 + V(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x). \quad (6) \]
The Hamiltonian \( H_0 = -(\hbar^2/2m) d^2/dx^2 \) governs the free motion of the particle, while \( V(x) \) is a 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), we must first of all discretize the continuous variables \( x \) and \( t \). If the motion essentially takes place inside a finite region, say \( -d \leq x \leq d \), we 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 \( \psi(x, t) \) is approximated by
\[ \sum_{k=0}^{2^n-1} c_k(t) |k\rangle = \frac{1}{\mathcal{N}} \sum_{k=0}^{2^n-1} \psi(x_k, t) |k\rangle, \quad (7) \]
where
\[ x_k \equiv -d + (k + \frac{1}{2}) \Delta, \quad (8) \]
\[ |k\rangle = |k_{n-1}\rangle|k_{n-2}\rangle \ldots |k_0\rangle \]
is a state of the computational basis of the \( n \)-qubit quantum register and
\[ \mathcal{N} = \sqrt{\sum_{k=0}^{2^n-1} \langle \psi(x_k, t) \rangle^2}. \quad (9) \]
is a factor that ensures correct normalization of the wave function. It is intuitive that (7) provides a good approximation to \( |\psi\rangle \) when the discretization step \( \Delta \) is much smaller than the shortest length scale relevant for the description of the system.

The Schrödinger equation (5) may be integrated formally by propagating the initial wave function \( \psi(x, 0) \) for each time-step \( \epsilon \) as follows:
\[ \psi(x, t + \epsilon) = e^{-\frac{i}{\hbar}H_0 \epsilon + V(x) \epsilon} \psi(x, t). \quad (10) \]
If the time-step \( \epsilon \) is small enough (that is, much smaller than the time scales of interest for the dynamics of the system), it is possible to write
\[ e^{-\frac{i}{\hbar}H_0 \epsilon} \approx e^{-\frac{i}{\hbar}H_0} e^{-\frac{i}{\hbar}V(x) \epsilon}. \quad (11) \]
Note that this equation, known as the Trotter decomposition, is only exact up to terms of order \( \epsilon^2 \) since the operators \( H_0 \) and \( V \) do not commute. The operator on the right-hand side of Eq. (11) is still unitary and simpler than that on the left-hand side. We can now take advantage of the fact that the Fourier transform can be efficiently performed by a quantum computer. We call \( p \) the momentum variable conjugate to \( x \), that is, \(-i\hbar \partial/dx = F^{-1} p F\), where \( F \) is the Fourier transform. Therefore, we can write the first operator in the right-hand side of (11) as
\[ e^{-\frac{i}{\hbar}H_0 \epsilon} = F^{-1} e^{-\frac{i}{\hbar}\left(\frac{p^2}{m}\right) \epsilon} F. \quad (12) \]
In this expression, we pass, by means of the Fourier transform \( F \), from the \( x \)-representation to the \( p \)-representation, in which this operator is diagonal. Then, using the inverse Fourier transform \( F^{-1} \), we return to the \( x \)-representation, in which the operator \( \exp(-iV(x)\epsilon/\hbar) \) is diagonal. The wave function \( \psi(x, t) \) at time \( t = l\epsilon \) is obtained (up to errors \( O(\epsilon^2) \)) from the initial wave function \( \psi(x, 0) \) by applying \( l \) times the unitary operator
\[ F^{-1} e^{-\frac{i}{\hbar}\left(\frac{p^2}{m}\right) \epsilon} \big| \psi(V(x) \epsilon) \big| F. \quad (13) \]

Therefore, simulation of the Schrödinger equation is now reduced to the implementation of the Fourier transform plus diagonal operators of the form
\[ |x\rangle \rightarrow e^{iF(x)} |x\rangle. \quad (14) \]
Note that an operator of the form (14) appears both in the computation of \( \exp(-iV(x)\epsilon/\hbar) \) and of \( \exp(-iH_0\epsilon/\hbar) \), when this latter operator is written in the \( p \)-representation. Any operator of the form (14) can be implemented by means of \( 2^n/2 \) generalized controlled-phase shift gates, which apply the transformation \( F_k \) to the target qubit only when the \( n-1 \) (control) qubits are in the state \( |k\rangle \). Here \( F_k \) is a single-qubit gate, mapping \( |0\rangle \) into the \( 2k \)th \( |0\rangle \) and \( |1\rangle \) into the \( 2k+1 \)th \( |1\rangle \). It is easy to check this construction for the three-qubit case shown in Fig. 2. \( F_0 \) acts only when the first two qubits are in the state \( |00\rangle \) and therefore it sets the phase \( e^{iF(0)} \) \( e^{iF(1)} \) \( e^{iF(3)} \) in front of the basis vectors \( |000\rangle \) and \( |001\rangle \), respectively. Similarly, \( F_1 \) acts only when the first two qubits are in the state \( |01\rangle \) and therefore it sets the phase \( e^{iF(2)} \) in front of the basis vectors \( |010\rangle \) and \( |011\rangle \) and so on.

Note that the implementation described in Fig. 2 is inefficient, as it scales exponentially with the number of qubits. On the other hand, efficient (that its, polynomial in \( n \)) implementations are possible for most of the cases of physical interest. For instance, \( n^2 \) two-qubit phase-shift gates are sufficient for the harmonic oscillator potential \( V(x) = \frac{1}{2} m \omega^2 x^2 \). Using Eqs. (8) and (2), we can write the discretized variable \( x \) as \( \alpha \sum_{j=0}^{n-1} (k_j 2^j + \beta) \), with the constants \( \alpha = \Delta \) and \( \beta = -d \Delta/\alpha n \). Therefore, \( x^2 = \)
standard projective measurement on the computational

gate run up to time $t$

Therefore, the probability distribution $\sum_{j,l=0}^{N-1}(k_j 2^j + \beta)(k_l 2^l + \beta)$ and finally

$$e^{-i\Phi V(x)}e = \prod_{j,l=0}^{n-1} e^{-i\gamma(k_j 2^j + \beta)(k_l 2^l + \beta)},$$

where $\gamma = m\omega^2 \alpha^2 \epsilon/(2\hbar)$. This is the product of $n^2$ phase-shift gates, each acting non-trivially (differently from identity) only on the qubits $j$ and $l$. Since the kinetic energy $H_0$ is proportional to $p^2$, an analogous decomposition is readily obtained, in the momentum eigenbasis, for $\exp(-iH_0\epsilon/\hbar)$. Efficient implementations are possible for piecewise analytic potentials $V(x)$ but require, in general, the use of ancillary qubits.

Finally, we point out that there is an exponential advantage in memory requirements with respect to classical computation. While a classical computer needs $O(N)$ bits to load the state vector of a system of size $N$ (that is, the coefficients $\psi(x_n,t)$ of its expansion over the computational basis), a quantum computer accomplishes the same task with just $n = \log_2 N$ qubits, namely with memory resources only logarithmic in the system size. As we have discussed in Sec. II, this is possible thanks to entanglement of the qubits in quantum computer.

V. A FEW SNAPSHOTs

To illustrate the working of the quantum simulator, we simulate it on a classical computer, obviously with an exponential slowing down with respect to a true quantum computation. Let us consider a few significant examples of single-particle quantum mechanical problems, for which plots of $|\psi(x,t)|^2$ are shown in Fig. 3. In contrast to classical simulations, in quantum computation we cannot access the wave function $\psi(x,t)$ after a single run up to time $t$. Indeed, each run is followed by a standard projective measurement on the computational basis, giving outcome $x_k$ with probability $|\langle k|\psi(x,t)\rangle|^2$. Therefore, the probability distribution $|\psi(x,t)|^2$ may be reconstructed, up to statistical errors, only if the quantum simulation is repeated many times. If outcome $x_k$ is obtained $N_k$ times in $N$ runs, we can estimate $|\psi(x_k,t)|^2$ as $N^2 N_k^2 / N^2$, with $N$ normalization factor defined in Eq. (9).

Fig. 3 exhibits several interesting features of quantum mechanics. In the top left plot we can see the spreading (quadratic in time) of a Gaussian wave packet for an accelerated particle. In the top right plot interference fringes appear when a Gaussian packet impinges on a square barrier. The bottom left plot shows the width oscillations for a squeezed state, back and forth between a minimum and a maximum value. Finally, the bottom right plot illustrates the motion of a wave packet in a potential harmonic for $x > 0$ and anharmonic ($V(x) = \alpha x^3$) for $x < 0$. We can see the deformation and spreading of the wave packet when it moves in the anharmonic part of the potential. As a result, the initial coherence of the state is lost in a couple of oscillation periods.

As shown in Fig. 4, it is also possible to measure the squares of the real and imaginary parts of $\psi(x,t)$. The line with a dash represents a set of $n$ qubits.
by means of a Ramsey type quantum interferometry method. For this purpose, we need a single ancillary qubit, initially in the state $|0\rangle$. The input state of the other $n$ qubits is $|0\rangle = |00\cdots0\rangle$ and they end up, depending on the $|0\rangle$ or $|1\rangle$ state of the ancillary qubit, in the states $|\psi(t)\rangle = W(t)|0\rangle$ or $|\psi^*(t)\rangle = W^*(t)|0\rangle$. Note that the operator $W(t) = U(t)S$ includes both the state preparation $|\psi(0)\rangle = S|0\rangle$ and the time evolution $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. Finally, a Hadamard gate applied to the ancillary qubit leads to the $(n+1)$-qubit output state

\[
|\Phi(t)\rangle = \frac{1}{2} |0\rangle (|\psi(t)\rangle + |\psi^*(t)\rangle) + \frac{1}{2} |1\rangle (|\psi(t)\rangle - |\psi^*(t)\rangle).
\]

(16)

Hence, the probabilities of obtaining outcomes 0 or 1 from the measurement of the ancillary qubit and $x_k$ from the measurement of the other $n$ qubits are given by

\[
P_0(x_k,t) = |\langle k|\Phi(t)\rangle|^2 = \{\text{Re} [\psi(x_k,t)]\}^2,
\]

(17)

\[
P_1(x_k,t) = |\langle 1|\Phi(t)\rangle|^2 = \{\text{Im} [\psi(x_k,t)]\}^2.
\]

(18)

From the measurement of $\{\text{Re} [\psi(x_k,t)]\}^2$ and $\{\text{Im} [\psi(x_k,t)]\}^2$ we can derive the phase velocity from the isophase curves of the wave function $\psi(x,t) = |\psi(x,t)| e^{i\phi(x,t)}$, corresponding to $\theta(x,t) = 0, \pi$ (implying $\text{Im} [\psi(x_k,t)] = 0$) and $\theta(x,t) = \frac{1}{2}\pi, \frac{3}{2}\pi$ (implying $\text{Re} [\psi(x_k,t)] = 0$). The phase velocity is just given by the slope of the isophase curves. In Fig. 5, $\{\text{Re} [\psi(x_k,t)]\}^2$ and $\{\text{Im} [\psi(x_k,t)]\}^2$ are shown for the quantum motion of a uniformly accelerated particle. It is interesting to note that in this example the phase velocity has strong local variations: it can change sign and also diverge.

The huge memory capabilities of the quantum computer appear in the plots of Fig. 6, where the dynamics of the superposition of two counterpropagating Gaussian packets in a harmonic potential is considered. When the two packets collide interference fringes appear, similarly to the double-slit experiment for free particles. These fringes are hardly visible with $n = 6$ qubits but already very clear with $n = 8$ qubits. Since the number of levels grows exponentially with the number of qubits, the discretization step reduces exponentially. Therefore, position resolution improves 4 times when moving from 6 to 8 qubits (of course, there is a lowest resolution limit imposed by the Heisenberg uncertainty principle).

Finally, we point out that the use of the quantum Fourier transform in the simulation of the Schrödinger equation automatically imposes periodic boundary conditions. Such boundary effects become relevant when the finite region $-d \leq x \leq d$ is not large enough for a correct description of the motion. This problem can be seen in the two top plots of Fig. 3. In the case of the uniformly accelerated particle, when the wave packet gets close to the upper border $x = +d$, there exists a spurious non-negligible probability to find the particle close to the lower border $x = -d$. With regard to the problem of the scattering of a particle by a square potential, we observe interference fringes between the transmitted and the reflected packets, when both are close to the boundaries.

VI. FINAL REMARKS

To assess the feasibility of a quantum computer, one should take into account that, in any realistic implementation, errors due to imperfections in the quantum computer hardware or to the undesired computer-environment coupling unavoidably appear. First studies\(^1,15\) have shown that a quantum simulator with $n = 6 - 10$ qubits is quite robust against errors. Nowadays, these numbers of qubits are available in experiments with liquid state nuclear magnetic resonance-based quantum processors and with cold ions in a trap\(^1\). On the other hand, the number of elementary quantum gates required for the simulations discussed in Figs. 3, 5, and 6 is $O(10^4)$, much larger than the sequences of $10 - 100$ gates that can be reliably imple-
mented in present-day laboratory experiments.

Even though the time when a useful quantum computer will be realized is uncertain, quantum computation is a very promising and fascinating field of investigation in physics, mathematics and computer science. Furthermore, we believe that quantum computation and more generally quantum information provide an excellent ap-


to teaching basic quantum mechanics, because they deal in an intuitive, appealing and mathematically simple way with the main features of the quantum theory, from the superposition principle to entanglement, quantum interference and quantum measurements.

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* Electronic address: giuliano.benenti@uninsubria.it
† Electronic address: giuliano.strini@mi.infn.it
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