Open Quantum Systems dynamics and quantum algorithms

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Abstract
The model of open quantum systems is adopted to describe the non-local dynamical behaviour of qubits processed by entangling gates. The analysis gets to the conclusion that a distinction between evaluation steps and task-oriented computing steps is justified only within classical computation. In fact, the use of entangling gates permits to reduce two steps (evaluation and calculation) to a single computational one, and this determines an effective computational speed-up. The application of the open quantum systems model suggests that the reduction to one-computational step is strongly related to the existence of Universal Dynamical Maps describing the evolution of component systems of two-qubits gates. As the description in terms of Universal Dynamical Map is possible only in the presence of a separable initial state, it turns out that the internal reduced dynamics with respect to entangling gates is neither unitary nor Markovian. The fact imposes a holistic vision on the structure of the algorithm, where the entangling gates shall remain indivisible units, or black boxes, in order to preserve computational speed as well as reversibility. This fact suggests to adopt a perspective on computation which is completely non-classical: the whole algorithm turns out not to be the sequence of its temporal parts.

1 Introduction
Quantum computation achievements are of fundamental importance on both physical and philosophical field. In 1994 [9] Peter Shor designed a quantum algorithm capable of performing a number of mathematical tasks, such as discrete logarithm and factoring, considered hard to compute by classical computers. The result is of great importance as, at present, no effective classical algorithm is available which is capable of factoring within a polynomial complexity-bound, which means, in an acceptable amount of time. On the contrary, Shor’s algorithm consists of a quantum procedure for factoring respecting such bound.

The quantum algorithm for factoring is based on the sequential application of three subalgorithms: two properly quantum ones, namely Quantum Fourier Transform (QFT) and Phase Estimation, and a classical one, Continued Fraction. It is a well known fact in the literature [6] that the achievement of a polynomial complexity-bound is made possible only by the application of QFT. However, it remains unanswered the reason why QFT turns out to be capable of working with such a low complexity-bound. In order to understand that, one usually compares QFT with the analogous most efficient classical algorithm, known as Fast Fourier Transform (FFT), which computes a Fourier transform following an exponential bound $O(n2^n)$. To understand why QFT allows a passage from exponential to polynomial bounds is the starting point of this work.

A quantum algorithm follows principles that differ from those of classical algorithms. In particular, the quantum approach imposes a revision of the concept of computation: dealing with quantum devices, for computation it is intended the physical dynamical evolution of physical objects, specifically the qubits. The logical operations performed on the qubits correspond to physical transformations of their quantum states.

Understanding the reason behind the sensational speed-up offered by QFT requires a close analysis of the internal structure of the QFT algorithm. In order to accomplish that, we apply the theoretical model of the Open Quantum Systems and consequently of dynamical maps, describing the evolution of single qubits processed during the computation.

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2 Computation as a dynamical process

A quantum algorithm is generally constituted by a set of standard elements: qubits, quantum channels, quantum logical gates and measurement apparatus. The qubits form the basic computational-unity. A crucial specification concerns the distinction between the qubit as a physical object (for example a photon or a spin), and its state (a vector or a density matrix in a Hilbert space), which are actually the storage and the carrier of the information, respectively.

In a quantum algorithm qubits move through apposite quantum channels. In principle, a channel may be thought of as the path covered by flying qubits, or as a chain of connected localized qubits, i.e. physical objects which are static along the structure of the channel, but whose state evolves in time by physical dynamics.

Logical operations consist of dynamical transformations of the qubits’ states and are carried out by quantum gates, which are unitary operators: gates may act on a single qubit or on two qubits.

The postulates of Quantum mechanics establish the association of the physical object encoding the qubit with a two-dimensional Hilbert space. Thus, the qubit’s state corresponds to a vector with two complex-components.

The action of a single-qubit gate corresponds to that of an operator on the Hilbert space of the qubit, and can be hence represented by a 2x2 matrix. The gate induces a dynamical evolution from an input to an output state. The dynamics takes place among two different times $t_0$ (initial or input) and $t^*$ (final or output). Introducing the input and output states, the action of the gate, see Fig.1, may be written as:

$$|\psi(t^*)\rangle = U_{Q_1}(t_0, t^*)|\psi(t_0)\rangle,$$

which suggests that the input and the output states are simply those describing the physical system associated to the qubit at two different times of its evolution.

$${|\psi_{in}\rangle := |\psi(t_0)\rangle,}$$

$${|\psi_{out}\rangle := |\psi(t^*)\rangle}.$$

Figure 1: equivalent representations of a one-qubit gate. The notation suggests the gate ($U_{Q_1}$) acts on the qubit $Q_1$ in the interval $[t_0, t^*]$.

The existence of a unitary operator ruling the evolution of a quantum state is guaranteed by quantum mechanics’ postulates:

$$|\psi(t)\rangle = U|\psi(0)\rangle,$$

with $UU^\dagger = 1$. On the other hand, by the unitary of $U$, it can be easily derived that there exists a Hermitian operator $K$ ($K^\dagger = K$), such that Eq.(4) may be written as:

$$|\psi(t)\rangle = e^{iKt}|\psi(0)\rangle.$$

$K$ normally corresponds to the Hamiltonian of the system, in particular it is $K = \frac{H}{\hbar}$. In Eq.(5) and throughout the paper, the Plank’s constant is set to unity.
One could argue that Eq. (5) is valid only in the case where $K$ is independent on time. This indeed holds true, as the independence of the Hamiltonian on time can be justified by assuming that the system is isolated. In fact, we should suppose the Hamiltonian being dependent on time only in presence of an external influence or interaction caused by another system. This does not occur in the case of a single-qubit gate, where the assumption of the time-independence of the Hamiltonian is hence justified.

Considering the dynamics of the single-qubit gate and setting $t_0 = 0$, one obtains:

$$U_{Q_1} = e^{-iKt^*},$$

which follows from the combination of Eq. (4) and Eq. (5) and defines the action of any single-qubit gate. Eq. (6) suggests that the action of the gate is strictly related with the instant $t^*$, which shall be fixed to set the gate for carrying out a specific task.

Let us consider, for instance, the gate $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, performing the spin-flip and corresponding to the Pauli operator $\sigma^x$. Writing

$$U_{Q_1} = e^{-iXt^*} = \sum_n \frac{(-it^*)^n}{n!} (X)^n =$$

$$= \left[ \sum_n \frac{-i(t^*)^{2n+1}}{(2n+1)!} (X)^{2n+1} + \sum_n \frac{(-it^*)^{2n}}{(2n)!} \right] 1 = i \sin(t^*) X - \cos(t^*) 1,$$

where we have used $X^{2n} = 1$ and $X^{2n+1} = X$, it is seen that the unitary dynamics corresponds to $X$ operation for $\sin(t^*) = 1$, i.e. for $t^* = \frac{\pi}{2} + 2k\pi$. Analogue reasoning can be carried on with respect to any local gate.

The above reasoning is justified under the crucial assumption that the system formed by the qubit and the gate is coupled with no environment, thus it is interpreted as isolated.

3 Dynamics of Open Quantum Systems and two-qubit gates

Two-qubit gates, and, in particular, two-qubit controlled gates (which are at the heart of quantum algorithms’ functioning), take one qubit as the control and the other as the target, on which the operation is actually implemented. In order to do that, the gate works on a composite system, and process simultaneously the states of the two qubits. The simultaneity permits to compute in a unique step the evaluation of the control qubit, and the specific operation on the target. As already discussed elsewhere [5], [3], [4], the physical resource imputable of allowing such a speed-up is entanglement.

The only physical way to represent the structure of a two-qubit gate is that of introducing a composite system, made of two subsystems. One assumes that the global composite system, say $S$, is isolated. On the contrary, as the aim of the gate is building (and consequently working with) entanglement, both subsystems shall be supposed to develop quantum correlations amongst each other, and consequently shall be assumed to be open.

Any two-qubit gate may be represented as a unitary operator acting on the Hilbert space of the composite system, which is the tensor product of the subsystems’ spaces. Therefore, if a gate acting on a single qubit may be represented as a 2x2 matrix, a two-qubit is written as a 4x4 one.

Two are the perspectives one may assume to describe the gate: a global one, see Fig.2, focusing on the action performed on the composite system $S$, and a local one, see Fig.3, based on the transformation induced on the two input qubits. In the first case, it is reasonable to sketch the action as a unitary operation on an initial tensor product state:

$$\rho_{in} = \rho_{Q_1}(t_0) \otimes \rho_{Q_2}(t_0).$$

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Figure 2: global perspective on the action of a two-qubit gate. It is $\rho_{in} = \rho_{Q_1}(t_0) \otimes \rho_{Q_2}(t_0)$ and $\rho_{out} = U\rho_{in}U^\dagger$. The notation suggests that the gate $U_{Q_1Q_2}$ acts simultaneously on qubits $Q_1$ and $Q_2$.

Considering the global system $S$ the action of the gate can be reduced to the single-qubit case. A more exhaustive analysis, however should clarify how to interpret the specific action of the gate on $Q_1$ and $Q_2$ separately; in other terms a local view on the dynamics should be considered. Let us describe the state of a single qubit, starting from the state of the composite system given in Eq. (9). This is obtained by introducing a reduced density matrix \[ \rho_{Q_1} = Tr_{Q_2} \rho. \] 

This can be done at any time of the evolution of the global system, so that:

\[ \rho_{Q_1}(t^*) = Tr_{Q_2} \rho_{out}. \]  

A local perspective imposes the description of the single qubit evolution and may be accomplished by introducing a dynamical map:

\[ \rho_{Q_1}(t^*) := \mathcal{E}_t[\rho_{Q_1}(t_0)]. \]  

The result of the local point of view is sketched in Fig.3.

Figure 3: local perspective on a two-qubit gate. The use of the colours stresses that it might be the case that qubits are entangled inside the gate and the output state can be entangled as well.

The form of the map $\mathcal{E}_t$ follows from the

**Theorem 3.1** Any kind of time-evolution of a quantum state $\rho_{Q_1}$ can be written in the form

\[ \rho_{Q_1}(t) = \sum_{\alpha} K_{\alpha}(t, \rho_{Q_1}(t_0)) \rho_{Q_1}(t_0) K_{\alpha}^\dagger(t, \rho_{Q_1}(t_0)), \]  

where $K_{\alpha}$ are Kraus operators depending on $t$ and state $\rho_{Q_1}$ at the initial time.

The action of the map is completely defined by the Kraus operators, for which important general properties hold (see [6]). The result of the above theorem is very general, i.e. it applies to any evolution of an open quantum system [11], but in our purposes, it underlines an existing problem, which turns out to be fundamental for computation: the dependence of Kraus operators on the initial state of the qubit. Let us look for maps, that are independent on the initial state of the system they act on: these are classified under the term Universal Dynamical Maps (UDM) and are definable imposing a relevant condition on the initial state of the composite system, according to the following

\[^{1}\text{All theorems’ proofs are skipped on purpose, as they can be found in literature (see [11]).}\]
Theorem 3.2 A dynamical map for \( Q_1 \) is a UDM iff it is induced from a composite system with the initial condition \( \rho(t_0) = \rho_{Q_1}(t_0) \otimes \rho_{Q_2}(t_0) \), and \( \rho_{Q_2}(t_0) \) fixed for any \( \rho_{Q_1}(t_0) \).

Theorems (3.1) and (3.2) represent two fundamental results for the study of open quantum systems dynamics \([8]\) \([11]\). From an epistemological point of view, it is interesting to underline that the definition of a UDM requires the separability of the global system’s state at the initial time. In other words, this means that the subsystems are set in pure states at the initial time, while they develop entanglement, thus acting as open, during the evolution.

4 Entangling gates

We have seen in the previous section that a two-qubit gate performs a non local action. For this reason, these gates are usually referred to as entangling gates \([2]\). An entangling gate is defined as an operator acting on a composite system, whose action cannot be written as a tensor product of two local operations:

\[
U_{\text{tot}} \neq U_{Q_1} \otimes U_{Q_2}
\]

In other terms, an entangling gate is considered as one capable of entangling at least one input state: it happens that the gate takes as input a tensor state and produces an output state, which cannot be written as a tensor product. The assertion can be exemplified referring to the C-phase gate,

\[
C_\phi = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i\phi}
\end{pmatrix}
\]

an example of a separable input state that gets "entangled" by the application of the gate can be easily sketched. In order to introduce the example, it is useful to remember the separability condition for the states of a two-qubit system. The most general two-qubit state is:

\[
|\Psi\rangle = \gamma_{00} |00\rangle + \gamma_{01} |01\rangle + \gamma_{10} |10\rangle + \gamma_{11} |11\rangle.
\]  

(16)

On the other hand, a separable state has the form:

\[
|\Psi\rangle_{\text{sep}} = (\alpha_0 |0\rangle + \alpha_1 |1\rangle)(\beta_0 |0\rangle + \beta_1 |1\rangle).
\]  

(17)

The combination of Eq.(16) and Eq.(17) shows that in order to have a separable state, the following relation among the coefficients \( \gamma_{ij} \) must hold:

\[
\frac{\gamma_{00}}{\gamma_{11}} = \frac{\gamma_{10}}{\gamma_{11}} = 1
\]

(18)

Let us now consider the separable state \( |\Psi\rangle = (|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle) \) (normalization is meaningless for the sake of simplicity), it is:

\[
C_\phi|\Phi\rangle = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i\phi}
\end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ e^{i\phi} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},
\]

(19)

for which the separability condition does not hold, being:

\[
\frac{\gamma_{00}}{\gamma_{11}} = 1 \neq \frac{\gamma_{10}}{\gamma_{11}} = \frac{1}{e^{i\phi}}.
\]

(20)

The example proves the existence of at least one separable state that, after having been processed, is entangled. However, it is not always the case that \( C_\phi \) produces entangled outputs. On this matter, the QFT algorithm represents a typical situation, such that C-phase gate is necessarily called to produce separable outputs. Such a requirement is forced by several reasons: firstly, because the entire algorithm is constituted by blocks, each one containing a sequential application of \( C_\phi \) gates, thus each output state is taken as input from another \( C_\phi \) and hence it shall be separable. Secondly, as the requirement of separability is fundamental for the "reading" process. Indeed, at the end of the algorithm the information...
stored in the qubits must be read out from a hypothetical user by performing measurements on the single qubits, and this requires the latter to be in a pure state.

The use of $C_\phi$ in the QFT is fundamental to build the desired Fourier transform. To give an idea of how the gate is capable of producing a separable output, we suppose the input state to be:

$$|\Phi\rangle = (|0\rangle + |1\rangle)_{Q_1}|q_2\rangle_{Q_2},$$  \hspace{1cm} (21)

setting the target in a superposition, while leaving the control undefined. It is easy to verify that:

$$C_\phi|\Phi\rangle = \begin{cases} 
(1 + e^{i\phi}|1\rangle)_{Q_1}|q_2\rangle_{Q_2}, & \text{if } q_2 = 0 \\
(0 + e^{i\phi}|1\rangle)_{Q_1}|q_2\rangle_{Q_2}, & \text{if } q_2 = 1 
\end{cases}$$  \hspace{1cm} (22)

At this point, one may argue that as the output consists of a separable state, no entanglement has occurred in the internal dynamics. A detailed analysis of the physical dynamics of the entangling gate would give the proof that the previous sentence is wrong. However, even without recurring to a detailed analysis of the dynamics, it is enough to check that the definition of entangling gate, given in Eq. (14), holds for $C_\phi$, which can not be constructed as the tensor product of the two local operations $1$ and $\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$:

$$C_\phi \neq 1 \otimes \phi.$$  \hspace{1cm} (23)

Eq. (23) contains a very relevant insight for our reasoning: if the gate is supposed to work in a time interval $[t_0, t^*]$, it must exist $t_1 \in [t_0, t^*]$ such that:

$$\rho_{Q_1, Q_2}(t_1) \neq \rho_{Q_1}(t_1) \otimes \rho_{Q_2}(t_1).$$  \hspace{1cm} (24)

Eq. (24) exemplifies the developing of entanglement inside the gate and forces to treat the system associated to the gate as open, implying its dynamics to be essentially non-Markovian [8]. In other terms, at the light of the theorem 3.2, it follows that no UDM is available to describe the evolution of $Q_1$ from any $t \in (t_0, t^*)$.

Figure 4: graphical representation of the non-Markovian character of UDM given in Eq. (24).

5 A perspective on entangling gates

A graphic representation of a quantum algorithm (see for example QFT in [6]) is visualized as a two-dimensional scheme. This is the result of a holistic perspective, i.e. it follows from looking at the algorithm from an external point of view. From such a perspective, the figure naturally calls for a sampling of the entire algorithm along two directions: horizontal and vertical.
The picture in Fig.5 fixes a possible partition of the structure of the algorithm. Different horizontal lines individuate the physical components, i.e. the qubits, while vertical lines stand to indicate a possible partition of the dynamical evolution. In other terms, we are able to accomplish both a time and a physical partition. Our interest is to individuate the existing relation between the whole and the time-parts as well as the physical parts.

Time-line is a continuous, thus the whole time-evolution of an algorithm can be divided into an arbitrary number of parts. Supposing to scan the algorithm in a decomposition that isolates all the entangling gates, we ask whether it is possible to divide further such gates. In other words, considering an entangling gate as a whole, a sort of black box, we inquire whether it is possible to investigate its internal dynamics as related to that of its internal parts.

Let us consider an entangling gate working between time $t_j$ and $t_{j+1}$. We ask ourselves whether we can describe its evolution in more details by a "refined time-sampling" of the operating interval $[t_j, t_{j+1}]$

$$[t_j, t_j + \varepsilon] \cup [t_j + \varepsilon, t_j + 2\varepsilon] \cup ... \cup [t_j - \varepsilon, t_{j+1}],$$

with $M\varepsilon = t_{j+1} - t_j$, for all $M \in \mathbb{N}$. As far as a black box is watched from an external perspective and thus considered as a whole, there is no problem in describing it at any time of the partition (25), using Schroedinger equation, although no information is gained on the qubits with respect to the mere knowledge of the global $U_{tot}$.

On the other hand, it is known that the gate operates on a composite system. Therefore, we are forced to break such system, into its open subsystems. In a strict sense, the black box remains exactly the same,
indeed the operator $U_{tot}$ is not substituted by another one. It is the observer’s perspective that changes. In the previous sections it has been stated that, in order to describe the evolution of a subsystem in terms of a UDM, it is necessary for the initial state of the composite system to be in a separable state, following the prescription of the theorem 3.2. On the other hand, we cannot renounce the idea of describing the evolution of a qubit under the effect of an entangling gate, via a map which does not depend on the initial state of the qubit itself. Indeed the work of the algorithm shall not depend on the input states, as this would make the concept of algorithm meaningless. The dependence of the map on the initial state implies that the former performs a preliminary evaluation on the qubit’s state, abandoning then the possibility of reducing evaluation and proper calculation (addition of a phase factor) to a unique step. In fact, as already mentioned, it is not by chance that the condition of separability, given in Eq. (9), is exactly verified at any application of entangling gates into the algorithm. If we consider the refined time-sampling of the gate dynamics from the local perspective, from Eq. (25) and Eq. (24), it follows that it must exist $t_j + m\varepsilon < t_{j+1}$, for some integer $m < M$, such that the qubit is entangled with its companion entering the gate; hence we cannot describe its evolution from $t_j + m\varepsilon$ to $t_{j+1}$ with a proper UDM. This establishes that the refined time-sampling is not possible. The above observation points out that the entangling gates are indivisible objects (figure below), hence they are not subjected to a potential “opening”. We believe such statement is stronger that the simple fact that “opening” the gate would imply the vanishing of the entanglement developed by the subsystems, but it is a natural consequence of the dynamical behaviours of open quantum systems, from which it follows that there exists no UDM mapping the qubits’ evolutions for internal times.

![Figure 7: representation of how entangling gates shall be interpreted in a quantum algorithm.](image)

The temporal indivisibility of some objects in a algorithm shows that the latter is not exactly the sequence of each temporal part. Comparing the two perspectives, one gets to the apparent paradox that the global dynamics is unitary and thus Markovian, while some portions of local dynamics are not. This imposes to state that an algorithm can not be considered neither as a composition nor as a sequence of its temporal parts. The above argument however has been derived using only one of the contents of theorem 3.2 and regards exclusively a possible temporal scan. To be more precise, it has been used only the condition about the separability of the initial state of the composite system. At this point, it is the case of considering also the physical parts as one might argue that the universality of the dynamical maps permits to apply exactly the same map to describe the evolution of both qubits $Q_1$ and $Q_2$ entering the gate. That is not the case and the reason follows from theorem 3.2, which in fact introduces a further condition for determining a UDM: the state of $Q_2$ at the initial time shall be fixed. This implies a certain dependence of the map acting on $Q_1$, on the state of $Q_2$, which in the case plays the role of an environment. In other words, both the evolutions of single qubits $Q_1$ and $Q_2$ may be mapped simultaneously by UDMs, but at cost of using two different ones namely $E_t^1$ and $E_t^2$ respectively.
The use of a different map for each qubit may lead one to think at the possibility of separating the two different objects entering the gate. Once more it can be shown that this would make the computation meaningless. Indeed, supposing that there exists a time \( t_2 \in [t_0, t^*] \), such that the qubits are found in a separable state
\[
\tilde{\rho} = \tilde{\rho}_{Q_1} \otimes \tilde{\rho}_{Q_2},
\]
implies the existence of two UDMs, one, namely \( E^{1}_{[t_0, t_2]} \), mapping the evolution in the interval \([t_0, t_2]\), and the other, \( E^{1}_{[t_2, t^*]} \), from \( t_2 \) to \( t^* \). The prescription of theorem (3.2) suggests that the two maps are different: indeed \( E^{1}_{[t_0, t_2]} \) is built basing on \( \rho_{Q_2} \) as environment for \( Q_1 \), while \( E^{1}_{[t_2, t^*]} \) on \( \tilde{\rho}_{Q_2} \), and
\[
\rho_{Q_2} \neq \tilde{\rho}_{Q_2},
\]
due to the action of the gate.

The above reasoning leads to the conclusion that an entangling gate behaves as a black box also, and especially with respect to any possible physical partition: the qubits may not be separated in any \( t \in [t_0, t^*] \). The fact implies that a quantum algorithm is not the mere juxtaposition of its physical parts.

In order to justify the relevant speed-up developed by a quantum algorithm, it is necessary to assume a holistic perspective on entangling gates, which is the only one plausible in order to preserve the UDM description.

6 Conclusions

Our discussion shows the existence of a dichotomy between the parts involved in the computation and the whole of an algorithm. Such a dichotomy relies on the structure of quantum algorithms and can neither be solved nor overcome.

Our analysis aimed at introducing the formal tools applied in the study of the open quantum systems to get some insights on the behaviours of entangling gates. The non-Markovian characters of such dynamics imposes the statement of a consistent divergence between quantum and classical computation. Indeed, assuming the Universal Turing machine as the model for classical computation, the machine can exploit the possibility of being stopped at any time of its evolution \[10,7\]; on the contrary, as our analysis pointed out, a quantum algorithm contains objects that cannot be divided in parts and this causes the impossibility of stopping the latter at any time.

Furthermore the consideration of the dichotomy leads us to state that the whole contains informations that can not be extracted from the parts. On the contrary, parts (physical-parts) constitute the strength of quantum computation, as they are imputable for the development of entanglement, however such a strength may be grabbed only by looking at entangling gates as a whole. In a few words, the requirement of speed-up has a high cost on the epistemic field: ignorance on the parts involved.

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