Natural majorization of the Quantum Fourier Transformation in phase-estimation algorithms

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Abstract

We prove that majorization relations hold step by step in the Quantum Fourier Transformation (QFT) for phase-estimation algorithms. Our result relies on the fact that states which are mixed by Hadamard operators at any stage of the computation only differ by a phase. This property is a consequence of the structure of the initial state and of the QFT, based on controlled-phase operators and a single action of a Hadamard gate per qubit. The detail of our proof shows that Hadamard gates sort the probability distribution associated to the quantum state, whereas controlled-phase operators carry all the entanglement but are immaterial to majorization. We also prove that majorization in phase-estimation algorithms follows in a most natural way from unitary evolution, unlike its counterpart in Grover’s algorithm.

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1 Introduction

Majorization theory emerges as the natural framework to analyse and quantify the measure of disorder for classical probability distributions [1] [2] [3] [4]. Majorization ordering is far more severe than the one proposed by standard Shannon entropy. If one probability distribution majorizes another, a set of inequalities must hold that constrain the former probabilities with respect to the latter. These inequalities entail entropy ordering, but the converse is not necessarily true. Quantum mechanically, majorization has proven to be at the heart of the solution of a large number of quantum information problems. It has been shown that majorization plays a fundamental role in topics like ensemble realization, conversion of quantum states via local operations and classical communication, and characterization of positive operator valued measurements [5].

Recently [6], a Majorization Principle has been formulated and checked in the efficient quantum algorithms known so far: the family of Grover algorithms and the family of quantum-phase estimation algorithms. More precisely, Grover’s [12] and Shor’s [13] algorithms operate in such a way that the probability distribution associated to the quantum state in the computational basis is majorized step by step until it reaches an optimal state. This property has been completely proven in the case of Grover’s algorithm for search of an item in an unstructured database. The algorithm is based on the iterative application of a unitary transformation. It is easy to see [6] that each of these transformations majorizes the probability distribution associated to the computational basis provided the initial state is symmetric. This step-by-step majorization progresses smoothly until the algorithm reaches the solution state after $O(\sqrt{N})$ operations, where $N$ is the number of entries in the database.

The case of phase-estimation algorithms, which include Shor’s factorisation algorithm, Simon’s algorithm, clock synchronisation and Kitaev’s algorithm for the Abelian stabiliser problem [15] is more subtle. The key ingredients in all these algorithms are the use of the quantum Fourier transformation operator (QFT) and the promise of a specific structure of the initial state. In [6] it was checked that the canonical form of the QFT majorizes step by step the probability distribution attached to the computational basis. Here we provide a complete proof of how the notion of majorization formulated in [6] explicitly operates in the special case of phase-estimation quantum algorithms, and how this notion is related to the efficiency shown by these algorithms.

One of our main purposes is to present an explicit and detailed proof of the following proposition: Majorization works step by step in the QFT of phase-estimation algorithms. The whole property is based on the following ideas: Hadamard operators act majorizing the probability distribution given the symmetry of the
quantum state, and such a symmetry is partially preserved under the action of both Hadamard and controlled-phase gates \[6\]. The mathematical formulation of these concepts will lead us to define an “H(i)-pair” as that pair of computational states that can be mixed by a Hadamard operator acting over the \(i\)-th qubit. Furthermore, we also work out a property concerning the way in which majorization emerges naturally from unitary evolution for this type of quantum algorithms.

In order to assess the significance of step by step majorization we have analyzed a series of further examples that will be presented in a separate publication \[7\]. First, we have analyzed a variant of Berstein-Vazirani algorithm \[8\] where a quantum algorithm is able to obtain the slope of a linear function defined on \(Z_N\) using only one query to the function. The efficient algorithm solving this problem is of interest because no entanglement is ever present along the computation, while majorization is verified. Second, we have considered the problem of determining the parity of a given function using oracle calls as introduced in ref. \[9\]. The quantum oracular algorithm proposed showed no speed-up as well as no step-by-step majorization. Third, we have studied the set of quantum adiabatic algorithms proposed by Farhi et al. The efficiency of these algorithms has been studied in detail for Grover’s problem showing that non-linear evolutions do lead to more efficient algorithms \[10\]. We have indeed checked that the efficient time-path is associated to step-by-step majorization while the non-efficient time-path is not. Finally, we have studied the recently proposed quantum random walk algorithm to solve a classicaly hard graph problem \[11\]. This algorithm also shows a step-by-step minorization-majorization cycle. These four instances of step-by-step majorization will be presented elsewhere but can be considered here as motivation for a link between majorization and efficiency.

We have structured the paper as follows. In Sec. 2 we review some concepts about majorization theory and how they relate to quantum algorithms. We develop in Sec. 3 some properties of majorization in phase-estimation algorithms and present in detail the main problem to be solved. In Sec. 4 we produce the proof for QFT step-by-step majorization. In Sec. 5 we analyse the way in which majorization arises in these algorithms and, finally, in Sec. 6 we collect our conclusions.

## 2 Majorization theory and its relation to quantum algorithms

Let us review the notion of majorization formulated in \[6\] for quantum algorithms. Let us consider two vectors \(\vec{x}, \vec{y} \in \mathbb{R}^d\) such that \(\sum_{i=1}^d x_i = \sum_{i=1}^d y_i = 1\), whose components represent two different probability distributions. We say that distri-
bution $\vec{y}$ majorizes distribution $\vec{x}$ (written as $\vec{x} \prec \vec{y}$) if, and only if, there is a set of probabilities $p_j$ and permutation matrices $P_j$ such that

$$\vec{x} = \sum_j p_j P_j \vec{y}. \tag{1}$$

This definition gives us the intuitive notion that the $\vec{x}$ distribution is more disordered than $\vec{y}$, because the former can be obtained from the latter making a probabilistically weighted sum over permutations of $\vec{y}$. There is an alternative definition of majorization which is often more practical. Consider the components of the two vectors sorted in decreasing order, written as $(z_1, \ldots, z_d) \equiv \vec{z} \downarrow$. We say that $\vec{y} \downarrow$ majorizes $\vec{x} \downarrow$ if, and only if, the following set of inequalities holds:

$$\sum_{i=1}^k x_i \leq \sum_{i=1}^k y_i \quad k = 1 \ldots d - 1. \tag{2}$$

A third way of defining majorization involves the use of doubly stochastic matrices. A real $d \times d$ matrix $D = (D_{ij})$ is said to be doubly stochastic if its entries are non-negative, and each row and column of $D$ sums to 1. We say that $\vec{y}$ majorizes $\vec{x}$ if, and only if, there exists a doubly stochastic matrix $D$ such that

$$\vec{x} = D \vec{y}. \tag{3}$$

The three given definitions can be proven to be equivalent [4].

Majorization can be related to quantum algorithms in the following way: let $|\psi_m\rangle$ be the pure state representing the register in a quantum computer at an operating stage labelled by $m = 0, 1 \ldots M - 1$, where $M$ is the total number of steps of the algorithm. We can naturally associate a set of sorted probabilities $p_x$, $x = 0, 1 \ldots 2^n - 1$ to this quantum state of $n$ qubits in the following way: decompose the register state in the computational basis, i.e:

$$|\psi^{(m)}\rangle = \sum_{x=0}^{2^n - 1} c_x^{(m)} |x\rangle, \tag{4}$$

where $\{|x\rangle \equiv |x_{n-1}, x_{n-2} \ldots x_0\rangle\}_{x=0}^{2^n-1}$ denotes the basis states in binary notation, and $x = \sum_{j=0}^{n-1} x_j 2^j$. The probability distribution associated to this state is

$$p_x^{(m)} = |c_x^{(m)}|^2 = |\langle x |\psi^{(m)}\rangle|^2 \quad x = 0, 1 \ldots 2^n - 1, \tag{5}$$

corresponding to the set of probabilities to find each possible output. A quantum algorithm will be said to majorize step by step this probability distribution iff [6]

$$p_x^{(m)} < p_x^{(m+1)} \quad \forall m = 1, \ldots, M. \tag{6}$$
In such a case, there will be a neat flow of probability directed to the values of highest weight, in a way that the probability distribution will be steeper and steeper as the time arrow goes on.

It is important to note that majorization is attached to a probability distribution defined on a specific basis. Although majorization is basis dependent, the basis where the final measurement closing the algorithm is performed is singled out. The computational basis is often the natural measurement basis to analyze majorization since it gives the probability distribution associated to an eventual measurement. We could stop the computation at some arbitrary time and find, if step-by-step majorization is holding, that the probability distribution is orderly approaching the final one. There may be instances, like the determination of parity, where the measurement basis is different from the naive computational basis. The relevant concept of majorization should then be analyzed in the physical measurement basis.

3 Majorization in phase-estimation quantum algorithms

Phase-estimation algorithms, initially introduced by Kitaev [16], form a family of efficient quantum algorithms [15] that include, for instance, Shor’s factoring algorithm and discrete logarithms [13]. Their relevance is due to the exponential gain in computational time over known classical algorithms. The basic problem to solve can be stated as follows. Given an unitary operator $U$ and one of its eigenvectors $|v\rangle$, estimate the phase of the corresponding eigenvalue $U|v\rangle = e^{-2\pi i \phi}|v\rangle$, $\phi \in [0,1)$ with $n$ qubits accuracy. An efficient solution was found in [15] and can be summarised in the following series of steps, represented by the quantum circuit of Fig. 1:

(i) Prepare the pure state $|\psi^{(i)}\rangle = |00\ldots\rangle|v\rangle$, where $|00\ldots\rangle$ will be called the register state and $|v\rangle$ is the source state where we have stored the eigenvector of the unitary operator $U$.

(ii) Apply Hadamard operators

$$U_H = \frac{1}{\sqrt{2}} (\sigma_1 + \sigma_3)$$

over all the qubits in the register state.

(iii) Apply bit-wise controlled $U^j$ gates over the $|v\rangle$ state as shown in the Fig 1, where each $U^j$ gate corresponds to the application of $j$ times the proposed $U$ gate with $j = 0, 1 \ldots n - 1$. 

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Fig. 1: Quantum circuit corresponding to the phase-estimation algorithm. Arrows at the end indicate measurements.

Fig. 2: Canonical decomposition of the QFT operator. By $U_j$ we denote the controlled gate $|0\rangle\langle 0| + e^{2\pi i/2^j}|1\rangle\langle 1|$. 
(iv) Apply the QFT operator

\[ QFT : |q\rangle \rightarrow \frac{1}{2^{n/2}} \sum_{q'=0}^{2^n-1} e^{2\pi i q q'/2^n} |q'\rangle \]  

over the register state.

(v) Make a measurement of the register state of the system. This provides with high probability the corresponding eigenvalue of \( U \) with the required precision.

Let us now go through the algorithm focusing on how the majorization of the computational basis probabilities evolves. The application of the Hadamard gates in step (ii) to the initial state produces a lowest element of majorization,

\[ |\psi^{(ii)}\rangle = 2^{-n/2} \sum_{x=0}^{2^n-1} |x\rangle |v\rangle , \]  

yielding to the probability distribution \( p^{(ii)}_x = 2^{-n} \forall x \). The outcome of the controlled \( U^j \) gates in step (iii) is the product state

\[ |\psi^{(iii)}\rangle = 2^{-n/2} \left( |0\rangle + e^{-2\pi i 2^{n-1} \phi} |1\rangle \right) \cdots \left( |0\rangle + e^{-2\pi i 2^n \phi} |1\rangle \right) |v\rangle = 2^{-n/2} \sum_{x=0}^{2^n-1} e^{-2\pi i x \phi} |x\rangle |v\rangle . \]  

As the action of these gates only adds local phases in the computational basis, the uniform distribution for the probabilities is maintained \((p^{(iii)}_x = 2^{-n} \forall x)\).

Verifying majorization for the global action of the QFT is straightforward. After step (iv) the quantum state becomes

\[ |\psi^{(iv)}\rangle = 2^{-n} \sum_{x,y=0}^{2^n-1} e^{-2\pi i x (\phi - y/2^n)} |y\rangle |v\rangle . \]  

We then have the probability distribution

\[ p_y^{(iv)} = \left| 2^{-n} \sum_{x=0}^{2^n-1} e^{-2\pi i x (\phi - y/2^n)} \right|^2 \forall y . \]  

Majorization between the initial (ii) and final (iv) states is verified [3], according to the definition in [2]. The remaining step (v) corresponds to a measurement whose output is controlled with the probability distribution \( p_y^{(iv)} \).

The quantum speed up in the phase-estimation algorithm is rooted in the efficient processing of the QFT. It is then essential to investigate whether the majorization property so far observed is also present within the QFT step by step.
4 Step-by-step majorization of the Quantum Fourier Transformation in the phase-estimation algorithm

The mathematical statement about QFT we need to prove reads:

**Theorem**

The QFT majorizes step by step the probability distribution calculated in the computational basis as used in the phase-estimation algorithms.

This theorem is seen to emerge from two facts. It is, first, essential that the initial state entering the QFT has a certain symmetry to be discussed. Second, the order of the action of Hadamard and controlled-phase gates maintains as much of this symmetry as to be used by the rest of the algorithm. More precisely, Hadamard gates take the role of majorizing the probability distribution if some relative phases are properly protected. Controlled-phase transformations do preserve such a symmetry.

We divide the proof in three steps: the first one will consist on a majorization lemma (here is where majorization enters), the second one will consist on a phase preserving lemma, and finally the third one will be the analysis of the controlled-phase operators in the QFT. As hinted above, we will observe that the only relevant operators for the majorization procedure are the Hadamard gates acting over the different qubits, while controlled-phase operators, thought providing entanglement, will turn out to be immaterial to majorization.

4.1 A lemma concerning majorization

Let us introduce the concept of “H(i)-pair”, central to this paper. Consider a Hadamard gate $U_{H,i}$ acting on qubit $i$ of the quantum register. In general, the quantum register would correspond to a superposition of states. This superposition can be organized in pairs, each pair being characterized by the fact that the Hadamard operation on qubit $i$ will mix the two states in the pair. Let us illustrate this definition with the example of a general quantum state of two qubits:

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$= (\alpha|00\rangle + \beta|01\rangle) + (\gamma|10\rangle + \delta|11\rangle)$$

$$= (\alpha|00\rangle + \gamma|10\rangle) + (\beta|01\rangle + \delta|11\rangle).$$

(13)
The second line corresponds to organizing the state as $H(0)$-pairs, because each pair shares the first qubit value. The third line, instead, organizes the state on $H(1)$-pairs, because each pair shares the second qubit value.

We can now formulate the following lemma:

**Majorization lemma**

Let $|\psi\rangle$ be a pure quantum state, written in the computational basis as

$$|\psi\rangle = \sum_{x=0}^{2^n-1} c_x |x\rangle,$$

(14)

with the property that the probability amplitudes of the computational $H(i)$-pairs differ only by a phase for a given qubit $i$.

Then, the probability distribution resulting from $U_{H,i}|\psi\rangle$ majorizes the one resulting from $|\psi\rangle$.

**Proof**

Consider a $n$-qubit pure quantum state $|\psi\rangle$ with the assumed property that the probability amplitudes of all the $H(i)$-pairs differ only by a phase for a given qubit $i$. This state can always be written in the following way:

$$|\psi\rangle = a_1 |0\ldots0^i\ldots\rangle + a_1 e^{i\delta_1} |0\ldots1^i\ldots\rangle + \cdots + a_{2^n-1} |1\ldots0^i\ldots\rangle + a_{2^n-1} e^{i\delta_{2^n-1}} |1\ldots1^i\ldots\rangle.$$  

(15)

This expression makes explicit that the amplitude for every pair of states that can be mixed by a Hadamard transformation on the qubit $i$ only differ by a phase. The Hadamard gate $U_{H,i}$ will mix all these pairs. The two states in every pair are equal in all their qubits except the $i$-th one. After the application of the $U_{H,i}$ we have

$$U_{H,i}|\psi\rangle = 2^{-1/2} (a_1 (1 + e^{i\delta_1}) |0\ldots0^i\ldots\rangle + a_1 (1 - e^{i\delta_1}) |0\ldots1^i\ldots\rangle + \cdots + a_{2^n-1} (1 + e^{i\delta_{2^n-1}}) |1\ldots0^i\ldots\rangle + a_{2^n-1} (1 - e^{i\delta_{2^n-1}}) |1\ldots1^i\ldots\rangle).$$  

(16)

We have to find a set of probabilities $p_j$ and permutation matrices $P_j$ such that

$$\begin{pmatrix}
|a_1|^2 \\
|a_1|^2 \\
\vdots \\
|a_{2^n-1}|^2 \\
|a_{2^n-1}|^2
\end{pmatrix} = \sum_j p_j P_j
\begin{pmatrix}
|a_1|^2 (1 + \cos \delta_1) \\
|a_1|^2 (1 - \cos \delta_1) \\
\vdots \\
|a_{2^n-1}|^2 (1 + \cos \delta_{2^n-1}) \\
|a_{2^n-1}|^2 (1 - \cos \delta_{2^n-1})
\end{pmatrix},$$

(17)
and the unique solution to this probabilistic mixture is

\[ p_1 = p_2 = \frac{1}{2} \]

\[
P_1 = \begin{pmatrix} 1 & & & \cdots & & 1 \\ & 1 & & & \cdots & \end{pmatrix} ; \quad P_2 = \begin{pmatrix} 0 & 1 & & & \cdots & 0 \\ 1 & 0 & & & \cdots & 1 \end{pmatrix} .
\]

The permutation matrix \( P_1 \) is nothing but the identity matrix and \( P_2 \) is a permutation of the probabilities of each pair which has undergone Hadamard mixing. This completes the proof. □

Note that we have made use of the majorization’s definition given in eq. (1) in this proof. Consequently, it has not been necessary to introduce any notion of sorting of the components of the probability distribution. Such a requirement would have involved an explicit knowledge of the factors \( a_i \) and \( \delta_i \) for all \( i \), which is unknown to us in principle.

The lemma we have proven states that Hadamard transformation do order probability distributions when the input state has a special structure, namely those amplitudes to be mixed only differ by a phase. This is the key element pervading the whole proof. Hadamard transformations and controlled-phase transformations carefully preserve such a structure when needed as we shall now see.

### 4.2 A lemma concerning phase preservation

**Phase preserving Lemma**

Let us consider a set of Hadamard gates \( \{U_{H,j}\} \) with \( j = 0, 1 \ldots n-1 \) such that each of them can act only once and a quantum state |\( \psi \rangle \) such that the probability amplitudes of the computational \( H(j) \)-pairs differ only by a phase \( \forall j \).

Then, after applying any Hadamard \( U_{H,i} \) operator from this set, the resultant state retains the property that the \( H(j) \)-pairs differ only by a phase \( \forall j \neq i \).

This lemma states the fact the QFT works in such a way that states to be mixed by Hadamard transformations only differ by a phase all along the computation, till the very moment when the Hadamard operator acts on it. In other words, the structure of gates is respectful with the relative weights of the \( H(i) \)-pairs.

To prove the above lemma we need to build some intuition. Let us first go into an example.
We start by introducing a new notation for the phases appearing in the source quantum state of eq. (10) to be operated by the QFT operator. Let us define

$$\beta_x \equiv -2\pi x \phi.$$ 

Then

$$|\psi^{(iii)}\rangle = 2^{-n/2} \sum_{x=0}^{2^n-1} e^{i\beta_x} |x\rangle.$$  \hspace{1cm} (19)

Note that, because $x = \sum_{i=0}^{n-1} x_i 2^i$, we have that

$$\beta_x = \sum_{i=0}^{n-1} -2\pi x_i 2^i \phi \equiv \sum_{i=0}^{n-1} x_i \alpha_i,$$  \hspace{1cm} (20)

where $\alpha_i \equiv -2\pi 2^i \phi$. As an example of this notation, let us write the state in the case of three qubits:

$$|\psi\rangle = \frac{1}{2^{3/2}} \left( |000\rangle + e^{i\alpha_2} |100\rangle + e^{i\alpha_1} |010\rangle + e^{i(\alpha_2+\alpha_1)} |110\rangle \right)$$

$$+ \frac{1}{2^{3/2}} \left( |001\rangle + e^{i\alpha_2} |101\rangle + e^{i\alpha_1} |011\rangle + e^{i(\alpha_2+\alpha_1)} |111\rangle \right) e^{i\alpha_0}. \hspace{1cm} (21)$$

We have factorised the $\alpha_0$ phase in the second line. Alternatively, we can choose to factorise $\alpha_1$

$$|\psi\rangle = \frac{1}{2^{3/2}} \left( |000\rangle + e^{i\alpha_2} |100\rangle + e^{i\alpha_0} |001\rangle + e^{i(\alpha_2+\alpha_0)} |101\rangle \right)$$

$$+ \frac{1}{2^{3/2}} \left( |100\rangle + e^{i\alpha_2} |110\rangle + e^{i\alpha_0} |011\rangle + e^{i(\alpha_2+\alpha_0)} |111\rangle \right) e^{i\alpha_1}, \hspace{1cm} (22)$$

or $\alpha_2$,

$$|\psi\rangle = \frac{1}{2^{3/2}} \left( |000\rangle + e^{i\alpha_1} |010\rangle + e^{i\alpha_0} |001\rangle + e^{i(\alpha_1+\alpha_0)} |011\rangle \right)$$

$$+ \frac{1}{2^{3/2}} \left( |100\rangle + e^{i\alpha_1} |110\rangle + e^{i\alpha_0} |101\rangle + e^{i(\alpha_1+\alpha_0)} |111\rangle \right) e^{i\alpha_2}, \hspace{1cm} (23)$$

In total, the initial state for three qubits can be factorised in this three different ways. This example shows that there are three different ways of writing the quantum state by focusing on a particular qubit. This property is easily extrapolated to the general case of $n$-qubits: we can always write the quantum state $|\psi^{(iii)}\rangle$ in $n$ different ways factorising a particular phase in the second line.

**Proof**

In the general case we can factorise the $\alpha_j$ phase so that the pure state is written as

$$|\psi\rangle = |\psi^{(iii)}\rangle = \frac{1}{2^{n/2}} \left( \left| 0\ldots 0^j \ldots \right\rangle + \ldots + e^{i\sum_{k\neq j} \alpha_k} \left| 1\ldots 0^j \ldots \right\rangle \right)$$

$$+ \frac{1}{2^{n/2}} \left( \left| 0\ldots 1^j \ldots \right\rangle + \ldots + e^{i\sum_{k\neq j} \alpha_k} \left| 1\ldots 1^j \ldots \right\rangle \right) e^{i\alpha_j}. \hspace{1cm} (24)$$
Then, the action of the $U_{H,j}$ transforms the state as follows

$$U_{H,j}|\psi\rangle = \frac{(1+e^{i\alpha_j})}{2^{(n+1)/2}} \left( |0\ldots 0\ldots \rangle + \ldots + e^{i\sum_{k\neq j} \alpha_k} |1\ldots 0\ldots \rangle \right)$$

$$+ \frac{(1-e^{i\alpha_j})}{2^{(n+1)/2}} \left( |0\ldots 1\ldots \rangle + \ldots + e^{i\sum_{k\neq j} \alpha_k} |1\ldots 1\ldots \rangle \right).$$  

(25)

It is now clear that this resulting state still preserves the symmetry property necessary to apply the phase preserving lemma to the rest of qubits $i \neq j$. The reason is that the effect of the operator has been splitting the quantum state in two pieces which individually retain the property that all the $H(i)$-pairs differ only by a phase for $i \neq j$. If we now apply another Hadamard operator over a different qubit $i$, each of these two quantum states splits in turn in two pieces

$$U_{H,i}U_{H,j}|\psi\rangle =$$

$$\frac{(1+e^{i\alpha_j})(1+e^{i\alpha_i})}{2^{(n+2)/2}} \left( |0\ldots 0\ldots 0\ldots \rangle + \ldots + e^{i\sum_{k\neq i,j} \alpha_k} |1\ldots 0\ldots 0\ldots \rangle \right)$$

$$+ \frac{(1-e^{i\alpha_j})(1+e^{i\alpha_i})}{2^{(n+2)/2}} \left( |0\ldots 1\ldots 0\ldots \rangle + \ldots + e^{i\sum_{k\neq i,j} \alpha_k} |1\ldots 1\ldots 0\ldots \rangle \right)$$

$$+ \frac{(1+e^{i\alpha_j})(1-e^{i\alpha_i})}{2^{(n+2)/2}} \left( |0\ldots 0\ldots 1\ldots \rangle + \ldots + e^{i\sum_{k\neq i,j} \alpha_k} |1\ldots 0\ldots 1\ldots \rangle \right)$$

$$+ \frac{(1-e^{i\alpha_j})(1-e^{i\alpha_i})}{2^{(n+2)/2}} \left( |0\ldots 1\ldots 1\ldots \rangle + \ldots + e^{i\sum_{k\neq i,j} \alpha_k} |1\ldots 1\ldots 1\ldots \rangle \right).$$  

(26)

(where we have assumed $i > j$). The register now consists of a superposition of four quantum states, each made of amplitudes that only differ by a phase. Further application of a Hadamard gate over yet a different qubit would split each of the four states again in two pieces in a way that the symmetry would again be preserved. This splitting takes place each time a particular Hadamard acts. Thus, all Hadamard gates operate in turn producing majorization while not spoiling the symmetry property needed for the next step. This completes the proof of the phase preserving lemma. $\square$

### 4.3 Analysis of the controlled-phase operators

It is still necessary to verify that the action of controlled-phase gates does not interfere with the majorization action carried by the Hadamard gates. Let us concentrate on the action of $U_{H,n-1}$, which is the first Hadamard operator applied in the canonical decomposition of the QFT. Originally we had

$$|\psi\rangle = \frac{1}{2^{n/2}} \left( |00\ldots \rangle + \ldots + e^{i\sum_{k\neq n-1} \alpha_k} |01\ldots \rangle \right)$$

$$+ \frac{1}{2^{n/2}} \left( |10\ldots \rangle + \ldots + e^{i\sum_{k\neq n-1} \alpha_k} |11\ldots \rangle \right) e^{i\alpha_{n-1}},$$  

(27)
where we have taken out the $\alpha_{n-1}$ phase factor. After the action of $U_{H,n-1}$ we get

$$U_{H,n-1}\psi = \frac{(1+e^{i\alpha_{n-1}})}{2(n+1)^{1/2}} \left( |00\ldots0\rangle + \cdots + e^{i\sum_{k\neq n-1} \alpha_k} |00\ldots1\rangle \right) + \frac{(1-e^{i\alpha_{n-1}})}{2(n+1)^{1/2}} \left( |10\ldots0\rangle + \cdots + e^{i\sum_{k\neq n-1} \alpha_k} |10\ldots1\rangle \right) \equiv |a\rangle + |b\rangle. \quad (28)$$

We repeat the observation made in the second step that the state resulting from the action of $U_{H,n-1}$ can be divided into a sum of two states, which we have called $|a\rangle$ and $|b\rangle$. For both of these two states the amplitudes of the $H(j)$-pairs $\forall j \neq n-1$ still differ only by a phase.

We can now analyse the effect of the controlled-phase operators. Notice, first, that any two controlled-phase operators acting over the same qubit commute, no matter what the phases and the control qubits are. This is a direct consequence of the diagonal form of these type of operators, written in the computational basis (see for example [17]). Consequently, we can focus on what happens after applying a general controlled-phase operator over a given qubit. For simplicity we will assume that it will act over the $(n-1)$-th qubit so it will be applied over the state $U_{H,n-1}\psi$ (the following procedure is easily extrapolated to the controlled-phase operators acting over the rest of the qubits). If the control qubit is the $l$-th one ($l \neq n-1$), the operator will only add phases over those computational states of (28) such that both the 1-th and the $l$-th qubits are equal to 1, so we see that it will only act effectively over part of the $|b\rangle$ state. Let us write $|b\rangle$ factorising the $l$-th phase

$$|b\rangle = \frac{(1-e^{i\alpha_{n-1}})}{2(n+1)^{1/2}} \left( |10\ldots0\rangle + \cdots + e^{i\sum_{k\neq l,n-1} \alpha_k} |10\ldots1\rangle \right) + \frac{(1-e^{i\alpha_{n-1}})}{2(n+1)^{1/2}} \left( |11\ldots0\rangle + \cdots + e^{i\sum_{k\neq l,n-1} \alpha_k} |11\ldots1\rangle \right) e^{i\alpha_l}. \quad (29)$$

It is now clear that we have only added a global phase in the second piece of $|b\rangle$, which can always be absorbed in a redefinition of the phase $\alpha_l$. Hence we see that no relevant change is made in the quantum state concerning majorization, because the amplitudes of the computational $H(j)$-mixable states $\forall j \neq n-1$ still differ only by a single phase. The action of controlled-phase operators only amounts to a redefinition of phases, which does not affect the necessary property for the majorization lemma to hold. We see that the needed phase redefinition can be easily made each time one of these operators acts over a particular qubit.

4.4 Summary of the proof

We can now collect the three pieces of our argument:
• Each Hadamard operation acting on a suitably symmetric state produces majorization.

• Each time a Hadamard operator is applied, the state splits into two states preserving the key property of the majorization lemma with respect to the remaining Hadamard operators.

• Controlled-phase operators only involve phase redefinitions, which are immaterial to majorization.

It then follows the property that QFT operator majorizes step by step the probability distribution in phase-estimation algorithms when the initial state is a set of states differing by phases. □

We would like to emphasise some relevant points emerging from our proof. Controlled-phase operators play no role on majorization, though they provide entanglement. Curiously, Hadamard operators act exactly in the complementary way, providing majorization without providing entanglement. It is also interesting to note that the majorization arrow in the quantum algorithm is based on two ingredients. On the one hand we have the special properties of the quantum state, and on the other hand we have the structure of the QFT. A QFT acting on an arbitrary state would fail to obey majorization. In particular a subsequent application of a QFT on the final state obtained above would operate a minorization of probabilities, till reaching the original state.

It is arguable that the proof we have presented depends on the specific decomposition of the QFT in terms of individual gates. The underlying quantum circuit is not unique and majorization may not be present in alternative decompositions. To clarify this point we have analyzed the decomposition of the QFT proposed in Ref. [18]. This circuit works in a different way, implementing first a series of gates that do not change at all the probability distribution and then a set of Hadamard operations that do verify step-by-step majorization. The result remains true that an alternative efficient QFT obeys step-by-step majorization.

5 Natural majorization and efficient quantum algorithms

We now turn to investigate further the way majorization has emerged in the phase-estimation algorithm as compared to majorization in Grover’s algorithm. This comparison was not performed in [6]. We shall see that both algorithms work in a rather different manner. Majorization is more “natural” in the former than in
the latter. This naturalness is attached to the absence or presence of off-diagonal contributions appearing along the unitary evolution.

For a search in an unstructured database of a particular item, the best known classical algorithm (which is simply the examination one by one of all the items in the database) takes asymptotically $O(2^n)$ steps in succeeding (where $2^n \equiv N$ is the number of entries)[12]. However, Grover was able to find a quantum mechanical algorithm that implements a quadratic speed-up versus the classical one (that is, Grover’s quantum algorithm takes asymptotically $O(2^n/2)$ steps). We will not enter into precise details of the construction of this quantum algorithm, and will only make few comments on the way it proceeds.

Grover’s algorithm [12] can be reduced to a two-dimensional Hilbert space spanned by the state we are searching $|m\rangle$ and its orthogonal $|m^\perp\rangle$[19]. The unitary evolution of the quantum state is given by the repeated application of a kernel which amounts to a rotation

$$K = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

where $\cos \theta = 1 - 2/2^n$. Other choices of kernels are also valid but the one here presented is the optimal one [20]. The initial state of the computation is an equal superposition of all the computational states, written as $|\psi\rangle = 2^{-n/2}|m\rangle + (1 - 2^{-n})^{1/2}|m^\perp\rangle$ in this 2-dimensional notation. For a given intermediate computation step the state $(\alpha, \beta)$ will be transformed to $(\alpha', \beta')$. If we wish to express the initial amplitudes in terms of the final ones, we have:

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha' \cos \theta + \beta' \sin \theta \\ -\alpha' \sin \theta + \beta' \cos \theta \end{pmatrix}.$$  

We now take the modulus squared of the amplitudes, obtaining:

$$|\alpha|^2 = \cos^2 \theta \ |\alpha'|^2 + \sin^2 \theta \ |\beta'|^2 + 2 \cos \theta \sin \theta \ \text{Re}(\alpha'^* \beta')$$
$$|\beta|^2 = \sin^2 \theta \ |\alpha'|^2 + \cos^2 \theta \ |\beta'|^2 - 2 \cos \theta \sin \theta \ \text{Re}(\alpha'^* \beta').$$

It is clear that if the interference terms were to vanish then majorization would follow in a straightforward way from these two relations. To see this, note that in such a case we could obtain the initial probability set from the final one according to the definition given in eq. [11] of majorization, with probabilities $p_1 = \cos^2 \theta$, $p_2 = \sin^2 \theta$ and permutation matrices $P_1 = I$ and $P_2 = \sigma_1$ (the last one is just the permutation matrix of the two elements). Majorization would then follow in a natural way from just unitary evolution. But this is not the case in Grover’s algorithm, because interference terms do not vanish. Yet it is proven that majorization
in Grover’s algorithm exists [6], although the way it arises is not so directly related to the unitary evolution in the way presented here.

Let us turn back to the majorization in the phase-estimation algorithm and its relation to unitary evolution. We write the initial state to be operated upon by a Hadamard gate acting over the $j$-th qubit as

$$|\psi\rangle = c_0 |0\ldots 0^j \ldots\rangle + c_j |0\ldots 1^j \ldots\rangle + \cdots + c_{2(n-1)-j} |1\ldots 0^j \ldots\rangle + c_{2n-1} |1\ldots 1^j \ldots\rangle,$$

(33)

where we are focusing on the $H(j)$-mixable coefficients. Applying the Hadamard gate over the $j$-th qubit we get

$$U_{H,j} |\psi\rangle = 2^{-1/2} (c_0 + c_j) |0\ldots 0^j \ldots\rangle + 2^{-1/2} (c_0 - c_j) |0\ldots 1^j \ldots\rangle + \cdots + 2^{-1/2} (c_{2n-1-j} + c_{2n-1}) |1\ldots 0^j \ldots\rangle + 2^{-1/2} (c_{2n-1-j} - c_{2n-1}) |1\ldots 1^j \ldots\rangle.$$

(34)

Inverting the relations in this last equation, we can find the initial probability amplitudes in terms of the final ones. For a given pair of amplitudes $c_{m-j}$ and $c_m$ we find

$$c_{m-j} = 2^{-1/2} \left( 2^{-1/2} (c_{m-j} + c_m) + 2^{-1/2} (c_{m-j} - c_m) \right),$$

$$c_m = 2^{-1/2} \left( 2^{-1/2} (c_{m-j} + c_m) - 2^{-1/2} (c_{m-j} - c_m) \right),$$

(35)

and making the square modulus we have

$$|c_{m-j}|^2 = \frac{1}{2} \left( |2^{-1/2} (c_{m-j} + c_m)|^2 \right) + \frac{1}{2} \left( |2^{-1/2} (c_{m-j} - c_m)|^2 \right) + \frac{1}{2} \text{Re} \left( (c_{m-j} + c_m)^* (c_{m-j} - c_m) \right),$$

$$|c_m|^2 = \frac{1}{2} \left( |2^{-1/2} (c_{m-j} + c_m)|^2 \right) + \frac{1}{2} \left( |2^{-1/2} (c_{m-j} - c_m)|^2 \right) - \frac{1}{2} \text{Re} \left( (c_{m-j} + c_m)^* (c_{m-j} - c_m) \right).$$

(36)

As in the Grover’s previous example, we observe that if interference terms disappeared majorization would trivially arise from this set of relations. In such a case, we would only have to choose the set of probabilities and permutation matrices of [15] to prove this property. But again we note that in general those interference terms do not disappear, so majorization does not usually arise in this natural way from the unitary evolution (exactly the same that happened in Grover’s algorithm). For those terms to disappear, there must exist very specific
properties for the coefficient $c_i$. It is a straightforward exercise checking that the interference vanish if and only if

$$c_{m-j} = a_{m-j}$$
$$c_m = a_{m-j}e^{i\delta_{m-j}},$$

where $a_{m-j}$ is real.

It is a remarkable fact that this is the case of phase-estimation algorithms. Recalling the lemmas from the previous sections, the interference terms will vanish also step-by-step, so in the case of phase-estimation algorithms, step-by-step majorization arises as a natural consequence of unitary evolution, something that does not happen in a general case. We also realize that the form of the quantum state to be applied to the QFT in eq. (10) is precisely the unique possible form for step-by-step natural majorization to appear. In a way we can say that previous steps in the algorithm prepare the state in this unique form.

Actually the test for natural majorization can be performed for any unitary operation acting over any quantum state and consequently for any quantum algorithm. To make this observation clear, let us write in matrix notation a unitary evolution of a general quantum state in an $N$-dimensional Hilbert space:

$$\begin{pmatrix} \alpha_1' \\ \vdots \\ \alpha_N' \end{pmatrix} = U \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix},$$

where $\alpha_i$ are the amplitudes for the initial state, $\alpha_i'$ the amplitudes for the final state, and $U$ corresponds to the $N \times N$ matrix of a general unitary evolution. Inverting this relation we can obtain the original amplitudes in terms of the final ones. Now, if we write $U^\dagger$ as

$$U^\dagger = \begin{pmatrix} u_{11} & \cdots & u_{1N} \\ \vdots & \ddots & \vdots \\ u_{N1} & \cdots & u_{NN} \end{pmatrix},$$

we can again calculate the square modulus of the original amplitudes obtaining

$$|\alpha_1|^2 = |u_{11}|^2|\alpha_1'|^2 + \cdots + |u_{1N}|^2|\alpha_N'|^2 \text{ + interference terms}$$

$$|\alpha_N|^2 = |u_{N1}|^2|\alpha_1'|^2 + \cdots + |u_{NN}|^2|\alpha_N'|^2 \text{ + interference terms}.$$
where $D$ is a doubly stochastic matrix such that $D_{ij} \equiv |u_{ij}|^2$. Recalling eq. (3) we conclude that the final probability distribution majorizes the original one, in a way that majorization arises in a natural way from the unitary evolution. This result is reminiscent of other applications of majorization theory in quantum mechanics. For instance, ensemble realization is rooted in doubly stochastic matrices of the above form: given a density matrix $\rho$ and a probability distribution $p_i$, there exist normalised quantum states $|\psi_i\rangle$ such that

\[ \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i | \]  

(42)

if and only if $(p_i) = D\lambda_\rho$, where $\lambda_\rho$ is the vector of eigenvalues of $\rho$ and $D_{ij} \equiv |u_{ij}|^2$, being $u_{ij}$ the elements of a unitary matrix $[5]$.

6 Conclusions

Our main results in this paper have been to provide an explicit and detailed proof that the Quantum Fourier Transformation implements step by step majorization in phase-estimation quantum algorithms, along with a comparison between the different way in which the notion of majorization [6] operates for the two families of efficient quantum algorithms known so far. Further work on other quantum algorithms (Bernstein-Vazirani problem, determinaiton of parity, quantum adiabatic evolution and quantum random walks for non-trivial graphs) that will be presented elsewhere [7] reinforces the link between step-by-step majorization and efficiency.

The proof of majorization for QFT is based on introducing the concept of Hadamard pair, $H(i)$-pair, and three lemmas. A $H(i)$-pair corresponds to any pair of states which can be mixed by a Hadamard transformation on the bit $i$. The three lemmas show that:

- A Hadamard gate acting on the bit $i$ of a given register carries out majorization provided the register is made of $H(i)$-pairs where the two states in the pair only differ by a phase.

- A Hadamard gate on a bit $i$ preserves the relative phase structure of $H(j)$-pairs for $j \neq i$.

- Controlled-phase gates do not affect the phase structure of any $H(i)$-pair.

Step-by-step majorization then follows since the Quantum Fourier Transformation only uses one Hadamard gate per qubit supplemented with immaterial
controlled-phase gates. The detailed way in which majorization takes place sug-
ggest introducing the concept of natural majorization, defined as a majorization
which follows from unitary evolution in the absence of off-diagonal terms. Natural
majorization controls phase-estimation algorithms but is not present in Grover’s
algorithm. A classification of quantum algorithms according to a naturalness cri-
terium for majorization can be performed. We note that this classification fur-
thermore corresponds to the well classification in terms of their efficiency. Natural
majorization might be a distinct feature of exponential quantum speed up.

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