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Unitary and Anti-Unitary Quantum Descriptions of the Classical Not Gate

Abstract Two possible quantum descriptions of the classical NOT gate are investigated in the framework of the Hilbert space $\mathbb{C}^2$: the unitary and the anti–unitary operator realizations. The two cases are distinguished interpreting the unitary NOT as a quantum realization of the classical gate which on a *fixed* orthogonal pair of unit vectors, realizing once for all the classical bits 0 and 1, produces the required transformations $0 \to 1$ and $1 \to 0$ (i.e., *logical quantum* NOT). The anti–unitary NOT is a quantum realization of a gate which acts as a classical NOT on *any* pair of mutually orthogonal vectors, each of which is a potential realization of the classical bits (i.e., *universal quantum* NOT). Although the latter is not completely positive, one can give an approximated unitary realization of the gate by appending an ancilla. Finally, we consider the unitary and the anti–unitary operator realizations of two important *genuine quantum gates* that transform elements of the computational basis of $\mathbb{C}^2$ into its superpositions: the *square root of the identity* and the *square root of the* NOT.

Keywords Quantum gates, universal quantum NOT, square root of the NOT, square root of the identity.

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1 Introduction

As well known the classical realization of the NOT gate is described by the Boolean function $\neg$ which transforms the bits $(0, 1)$ according to the correspondences $0 \xrightarrow{\neg} 1$ and $1 \xrightarrow{\neg} 0$.

From the pure point of view of quantum logic, the quantum version of the classical NOT gate (see for instance [1], [2]) is described by an operator from the class $\mathcal{U}(\mathbb{C}^2)$ of all unitary operators on the single qubit Hilbert space $\mathbb{C}^2$.

(QL) For a given orthonormal basis $\mathcal{B} = \{|u_0\rangle, |u_1\rangle\}$ of the Hilbert space $\mathbb{C}^2$, the unitary operator $U_\mathcal{B} = |u_0\rangle\langle u_1| + |u_1\rangle\langle u_0|$ realizes the required transformations of the unit vector $|u_0\rangle$ into the unit vector $U_\mathcal{B}|u_0\rangle = |u_1\rangle$ and of the unit vector $|u_1\rangle$ into the unit vector $U_\mathcal{B}|u_1\rangle = |u_0\rangle$. Formally,

$$\forall \mathcal{B} = \{u_0, u_1\} \ \exists U_\mathcal{B} \in \mathcal{U}(\mathbb{C}^2) : |u_0\rangle \xrightarrow{U_\mathcal{B}} |u_1\rangle \text{ and } |u_1\rangle \xrightarrow{U_\mathcal{B}} |u_0\rangle \quad (1)$$

Note that in terms of density operators, the transitions of (1) are extended into the following ones:

$$\rho_{|u\rangle} \xrightarrow{\mathcal{U}_{|u\rangle}} U_{|u\rangle}\rho_{|u\rangle}U_{|u\rangle}^{-1} = \rho_{|u^\perp\rangle} \xrightarrow{\mathcal{U}_{|u\rangle}} (U_{|u\rangle})^2 \rho_{|u\rangle}(U_{|u\rangle}^{-1})^2 = \rho_{|u\rangle} \quad (2)$$

Fixed the *computational* basis $\mathcal{B}$, the unit vectors (states) $|u_0\rangle$ and $|u_1\rangle$ are the quantum representatives of the classical bits 0 and 1, respectively, and the (1) formalizes the right requirement of the quantum version of a NOT gate. Of course, it is not required (and in general this operator does not make) the same transformation for any other orthonormal basis $\{|w_0\rangle, |w_1\rangle\}$ of $\mathbb{C}^2$. The formulation (1) is a particular case of the general situation summarized in the following two points:

(S-OG) The *single vector orthogonality* condition

$$\forall |u\rangle \ \exists U_{|u\rangle} \in \mathcal{U}(\mathbb{C}^2) : \langle u|U_{|u\rangle}u\rangle = 0 \quad (3)$$

(SR) The *self–reversibility* condition $(U_{|u\rangle})^2 = \mathbb{I}$, which can be reformulated as $(U_{|u\rangle})^{-1} = U_{|u\rangle}$.

where the first *orthogonality* condition (S-OG) says that the pair of unit vectors $|u\rangle$ and $|u^\perp\rangle := U_{|u\rangle}u$ constitutes an orthonormal basis of $\mathbb{C}^2$ and the second one describes the expected behavior of a quantum NOT gate. The orthogonality condition can be geometrically characterized in the following way. If the density operator (pure state) $\rho_{|u\rangle}$ is represented by the real triple (P_x, P_y, P_z) on the surface $S_1(\mathbb{R}^3)$ of the Poincaré/Bloch (from now on Poincaré) unit sphere the transformation in $\mathcal{TC}_1^+(\mathbb{C}^2)$ of the state $\rho_{|u\rangle}$ into the state $\rho_{U_{|u\rangle}|u\rangle}$ corresponds in $S_1(\mathbb{R}^3)$ to the transformation of the original point $\mathbf{n} = (P_x, P_y, P_z)$ into its *antipodal* $-\mathbf{n} = (-P_x, -P_y, -P_z)$. For this reason, in the literature the transition $|u\rangle \to |u^\perp\rangle$ is also denoted as $|\mathbf{n}\rangle \to |-\mathbf{n}\rangle$.

Starting from the orthogonality condition alone, recently a certain number of contributions [4], [5], [6], [7], [8] has been published about a totally different formulation which consists in the following *universal* requirement:

(U-OG) whether it is possible to construct a *unique* operator which transforms *any* unit vector $|\psi\rangle \in \mathbb{C}^2$ into its orthogonal unit vector (up to a phase factor) performing in this way in the Poincaré sphere the transformation of any point on its surface into its antipodal. This can be formalized by the following *universal* orthogonality requirement:

$$\exists \Theta \; \forall |\psi\rangle , \; \langle \psi | \Theta \psi \rangle = 0 \tag{4}$$

This is a quite different situation from the one formalized by (3). Indeed, in the (S-OG) case the statement is of the form "for any ($\forall$) fixed vector, there exists ($\exists$) an operator such that (...)", whereas in the present (U-OG) case we have to do with a statement of the *universal* form "there exist ($\exists$) an operator, such that for every ($\forall$) vector (...)". Thus, operators of the latter case are called mathematical representations of the quantum *universal* NOT *gate* (U–NOT), differently from the former case of the simple *logical* NOT *gate* (L–NOT).

Of course, "it is not a problem to complement a classical bit, i.e., to change a value of a bit, a 0 to a 1 and vice versa. This is accomplished by a NOT gate"[4]. Similarly, from the quantum point of view if "complementing" (or *flipping*) an *a priori known* qubit means the choice of a (specific) state $|u\rangle$ and to transform it into its orthogonal state $|u^\perp\rangle$, then according to (1) this is done by the unitary L–NOT operator $U_{|u\rangle}$. But, if "the question we want to address is: Is it possible to build a device that will take an *arbitrary* (unknown) qubit and transform it into the qubit orthogonal to it? [Then] *complementing a qubit* (i.e., inverting the state of the spin–1/2 particles), [...] is another matter" [4].

A positive answer to this problem has been given by BHW in [4] by an anti–unitary operator $\Theta_{|u\rangle}$ defined, using an orthonormal basis $\mathcal{B} = \{|u\rangle , |u^\perp\rangle\}$ of $\mathbb{C}^2$, by its action on the generic vector $|\psi\rangle \in \mathbb{C}^2$ given by $\Theta_{|u\rangle} |\psi\rangle = \langle u^\perp |\psi\rangle^* |u\rangle - \langle u|\psi\rangle^* |u^\perp\rangle$. The interesting point is that for any arbitrary vector $|\psi\rangle$, whatever be the unit vector $|u\rangle$ (and so the basis $\mathcal{B}$), it is $\Theta_{|u\rangle} |\psi\rangle = |\psi^\perp\rangle$ since $\langle \psi | \Theta_{|u\rangle} \psi \rangle = 0$ holds. In the sequel we denote by $\mathcal{A}(\mathbb{C}^2)$ the class of all anti–unitary operators on $\mathbb{C}^2$.

Summarizing, "the problem is that one cannot flip a spin of unknown polarization. Indeed, it is easy to see that the *flip operator* defined as

$$\left[\exists \Theta \; \forall \mathbf{n} \in S_1(\mathbb{R}^3)\right], \; \Theta |\mathbf{n}\rangle = |-\mathbf{n}\rangle \tag{5}$$

is not unitary but anti–unitary. Thus there is no physical operation which could implement such a transformation" [5]. As usual in some physical tradition, in the just quoted original statement no mention is done about the exact role of the quantifiers $\exists, \forall$, and this is the reason of the part under the square brackets inserted by us. Anyway, this polar formulation (5) is trivially equivalent to the original (U-OG) formalized by (4).

From the formal point of view, the BHW anti-unitary operator $\Theta_{|u\rangle}$ satisfies something more than the above condition of universal orthogonality (U-OG), since it verifies:

(W-OG) The *universal orthogonality* (or *flipping*) condition

$$\forall |u\rangle \; \exists \Theta_{|u\rangle} \in \mathcal{A}(\mathbb{C}^2) : \forall |\psi\rangle , \; \langle \psi | \Theta_{|u\rangle} \psi \rangle = 0$$

(A-SR) The *anti self–reversibility* condition $\Theta_{|u\rangle}^2 = -\mathbb{I}$, which can be reformulated as $\Theta_{|u\rangle}^{-1} = -\Theta_{|u\rangle}$.

With respect to the linear case the transitions (1) are substituted by the transitions true for any $|\psi\rangle$

$$|\psi\rangle \xrightarrow{\Theta_{|u\rangle}} \Theta_{|u\rangle} |\psi\rangle \xrightarrow{\Theta_{|u\rangle}} \Theta_{|u\rangle}^2 |\psi\rangle = - |\psi\rangle \tag{6}$$

whose extensions to density operators are obtained by the von Neumann–Lüders operation $\mathcal{T}_{|u\rangle} := \Theta_{|u\rangle} \, (\, \cdot \,) \, \Theta_{|u\rangle}^{-1}$ according to:

$$\rho_{|\psi\rangle} \xrightarrow{\mathcal{T}_{|u\rangle}} \Theta_{|u\rangle} \, \rho_{|\psi\rangle} \, \Theta_{|u\rangle}^{-1} = \rho_{|\psi^\perp\rangle} \xrightarrow{\mathcal{T}_{|u\rangle}} \Theta_{|u\rangle}^2 \, \rho_{|\psi\rangle} \, (\Theta_{|u\rangle}^{-1})^2 = \rho_{|\psi\rangle} \tag{7}$$

From now on, for the sake of simplicity, we will consider the fixed computational basis $\mathcal{B}_c = \left\{ |0\rangle = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix} \right), |1\rangle = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix} \right) \right\}$ of $\mathbb{C}^2$ as concrete realization of the orthogonality pair $\{|u\rangle, |u^\perp\rangle\}$ and as qubit description of the Boolean classical bits 0 and 1. Then, denoted a vector on the unit surface $S_1(\mathbb{R}^3)$ with its polar representation $\mathbf{n} = (\sin\vartheta \cos\varphi, \sin\vartheta \sin\varphi, \cos\vartheta) \equiv (\vartheta, \varphi)$, the generic unit vector of $\mathbb{C}^2$ and its orthogonal can be represented as the pair

$$|\mathbf{n}\rangle = \begin{pmatrix} e^{-i\frac{\varphi}{2}} \cos\frac{\vartheta}{2} \\ e^{i\frac{\varphi}{2}} \sin\frac{\vartheta}{2} \end{pmatrix} \qquad |-\mathbf{n}\rangle = \begin{pmatrix} e^{-i\frac{\varphi}{2}} \sin\frac{\vartheta}{2} \\ -e^{i\frac{\varphi}{2}} \cos\frac{\vartheta}{2} \end{pmatrix} \tag{8}$$

with $\langle \mathbf{n} \, | - \mathbf{n} \rangle = 0$, whose Poincaré surface representations are just the two mutually antipodal points $\mathbf{n}$ and $-\mathbf{n}$.

The BHW anti–unitary realization of the U–NOT gate, in this context simply denoted by Θ instead of $\Theta_{|0\rangle}$, is characterized by the transition $\left(\begin{smallmatrix} c_0 \\ c_1 \end{smallmatrix} \right) \xrightarrow{\Theta} \left(\begin{smallmatrix} c_1^* \\ -c_0^* \end{smallmatrix} \right)$, whatever be the input vector from $\mathbb{C}^2$ or, making reference to (8), by the transition $|\mathbf{n}\rangle \xrightarrow{\Theta} |-\mathbf{n}\rangle$.

Coming back to the orthogonality condition, we have two possible strategies.

1.1 The unitary strategy

Let us stress that a variation of the unitary operator of the kind (1), in the present notation the unitary operator $N_1 = |0\rangle \langle 1| - |1\rangle \langle 0|$, actually stays in an intermediate position between the two above discussed versions (S-OG) and (U-OG). Of course, it is not a description of a unitary universal NOT gate, but it "complements" a lot of orthonormal pairs of states. Precisely, all the input states with real components, or equivalently all the orthonormal pairs of the type (8) satisfying the condition $\varphi = 0$, with ϑ ranging into the real interval $[0, 2\pi)$.

From the polarization interpretation of unit vectors of $\mathbb{C}^2$, the unitary operator N_1 can be considered *partially universal* in the sense that it transmits any (pure or mixed) state of *linear* polarization into its orthogonal state of *linear* polarization. But this does not happen in the case, for instance, of circular or elliptic polarization states.

1.2 The anti–unitary strategy

Of course, there could be another strategy based on the BHW anti–unitary operator which is a *universal* NOT transmitting any polarization state into its orthogonal (for instance also circular or elliptic polarization states). The strategy is to approximate an anti-unitary transformation on the two–dimensional Hilbert space $\mathbb{C}^2$ by a unitary transformation on a larger Hilbert space. Quoting [6]:"This operation is anti–unitary and therefore cannot be realized exactly. *So, how well we can do?* We find a unitary transformation acting on an input qubit and some auxiliary qubits, which represent degrees of freedom of the quantum NOT gate itself, which approximately realizes the NOT operation on the state of the original qubit. We call this 'device' a *universal*–NOT because the size of the error it produces is independent of the input state."

Formally, and without entering in technical details which can be found in the just quoted BHW paper, the procedure can be summarized in the following steps:

(St1) One considers the dynamical evolution of an *open* quantum system as the result of an interaction between the system under consideration described inside the system Hilbert space $\mathbb{C}^2$ and an additional one (the *reservoir*) described by the *ancilla* Hilbert space $\mathcal{H}_a$.
       The resulting system is a *closed* quantum system whose dynamical evolution must be described by a unitary operator on the tensor product Hilbert space $\mathbb{C}^2 \otimes \mathcal{H}_a$.

(St2) The action gate on the basis vectors $\{|0\rangle, |1\rangle\}$ of the Hilbert space $\mathbb{C}^2$ is described by the two following rules of some operator W on the Hilbert space $\mathbb{C}^2 \otimes \mathcal{H}_a$.

$$|0\rangle |Q\rangle \overset{W}{\mapsto} |1\rangle |Q_0\rangle + |0\rangle |Y_0\rangle \qquad (9\text{a})$$

$$|1\rangle |Q\rangle \overset{W}{\mapsto} |0\rangle |Q_1\rangle + |1\rangle |Y_1\rangle \qquad (9\text{b})$$

where $|Q\rangle$ describes the known states in which the ancilla is originally prepared, and $|Q_i\rangle$ and $|Y_i\rangle$ some ancilla output states which must be determines by suitable conditions. In particular the unitary condition on W determines some constraints on these vectors.

(St3) The input global state $|\Psi\rangle^{in} = |\psi\rangle |Q\rangle$ (in the Hilbert space $\mathbb{C}^2 \otimes \mathcal{H}_a$) constituted by the general system input state $|\psi\rangle = \cos\vartheta |0\rangle + e^{i\varphi} \sin\vartheta |1\rangle$ and the ancilla state $|Q\rangle$, under the conditions (9) and the linearity of the operator W, produces the transition:

$$|\psi\rangle |Q\rangle \overset{W}{\mapsto} |\Psi\rangle^{out} = \cos\vartheta \big(|1\rangle |Q_0\rangle + |0\rangle |Y_0\rangle \big) + e^{i\varphi} \sin\vartheta \big(|0\rangle |Q_1\rangle + |1\rangle |Y_1\rangle \big)$$

(St4) It is constructed the global output density operator $\rho_{|\Psi\rangle^{out}}$ on $\mathbb{C}^2 \otimes \mathcal{H}_a$ and its partial traced system density operator $\big(\rho_{|\Psi\rangle^{out}}\big)_s$ on $\mathbb{C}^2$, both depending from the parameters ϑ and φ which characterized the generic system input vector $|\psi\rangle$.

(St5) Then one calculates the fidelity of the system output state $\left(\rho_{|\Psi\rangle^{out}}\right)_s$ with respect to the output state $\psi^\perp \in \mathbb{C}^2$ expected as the result of the transition $|\psi\rangle \xrightarrow{\Theta} |\psi^\perp\rangle$ performed by the BHW anti–unitary operator:

$$F(\vartheta, \varphi) = \left\langle \psi^\perp \right| \left(\rho_{|\Psi\rangle^{out}}\right)_s \left| \psi^\perp \right\rangle$$

(St6) The important requirement is now that the fidelity must be independent from ϑ and φ in order to obtain a result which involves all the system input vectors.

This result is obtained imposing first the vanishing of the coefficients of all terms with a particular kind of φ dependence, and then demanding the vanishing of the remaining terms depending from ϑ. These conditions lead to the fidelity (independent from the angle pair ϑ and φ, and so true for any arbitrary system input vector $|\psi\rangle$):

$$F = ||Q_0||^2 = 1 - ||Y_0||^2$$

So, in order to maximize F we have to minimize $||Y_0||^2$, in such way that for any system input pure state $|\psi\rangle$ the system output state is "as close as possible" to the orthogonal qubit state $\Theta |\psi\rangle = |\psi^\perp\rangle$. This leads to the results that the ancilla Hilbert space is three dimensional, $\mathcal{H}_a = \mathbb{C}^3$, and that the vectors appearing in the (9) can be taken to form the orthonormal basis:

$$|Q_0\rangle = \sqrt{\frac{2}{3}} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |Q_1\rangle = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |Y_0\rangle = \sqrt{\frac{1}{3}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The corresponding fidelity is then $F = 2/3$.

1.3 The comparison of the two strategies

In summary,

1. the quantum logical L–Not gate N_1 has the positive aspect to be unitary, but with the drawback of performing only a partial, also if great (the cardinality of the continuum), number of orthogonal complementations (all the photon states of linear polarization);

2. the BHW gate Θ gives a positive answer to the full complementing requirement, i.e., it realizes the quantum universal U–Not gate, but with the drawback of being unphysical. However, it is possible, by appending a three dimensional auxiliary ancilla to the input qubit, to realize a unitary operator on the larger system which, partial traced on the system, furnishes the required transformations performed by the BHW gate with an approximation (the "size" of the error) quantified by the fidelity $2/3$, independent of the input state.

Let us stress that in this paper we don't treat this approximated realization of the universal NOT gate, but we are particularly interested to formalize the procedure of constructing both the linear and the anti–linear unitary realization of any classical n-in/n-out reversible gate, applying it to the particular case of the classical NOT gate obtaining in this way the usual unitary quantum NOT gate and the anti–unitary quantum BHW operator.

1.4 The non–linear versions of the square root of the Identity and of the NOT gates

In section 5, the unitary and anti–unitary versions of the square root of the NOT and of the square root of the identity gates are investigated. This is obtained simply applying by analogy the previously discussed procedure, in particular to both the unitary and the anti–unitary versions of the NOT gate which cannot be either unitary or anti–unitary, and so a specific solution is given by non–linear operators.

This result can be inserted in an investigation about non–linear quantum mechanics. As well as the work of Beltrametti and Bugajski [11], [12], [13], [14] and Bugajski [15], there have also been attempts to incorporate non–linear operators in quantum mechanics by, amongst others, Mielnik [16], [17], [18], Haag and Bannier [19] and Weinberg [20], [21]. In the just quoted non–linear contributions to quantum mechanics the non–linearity is applied to the case of observables, which in general are not additive ($\exists |\psi\rangle$, $|\phi\rangle$ s.t. $A(|\psi\rangle + |\phi\rangle) \neq A |\psi\rangle + A |\phi\rangle$), but satisfies either the homogeneity ($\forall |\psi\rangle$, $\forall \alpha \in \mathbb{C}$, $A\alpha |\psi\rangle = \alpha A |\psi\rangle$), or the anti–homogeneity ($\forall |\psi\rangle$, $\forall \alpha \in \mathbb{C}$, $A\alpha |\psi\rangle = \alpha^* A |\psi\rangle$), or the absolute homogeneity ($\forall |\psi\rangle$, $\forall \alpha \in \mathbb{C}$, $A\alpha |\psi\rangle = |\alpha| A |\psi\rangle$) (see for instance [22]). In this paper we obtain non–linear realizations of unitary operator which are both additive, but neither homogeneous, nor anti–homogeneous, nor absolutely homogeneous.

2 Quantum gate description of Boolean gate: semi–classical quantum gates

Computational models are usually based upon Boolean logic, and use some universal set of primitive connectives such as, for example, {AND, NOT}. From a general point of view, a *classical (Boolean) n–input/m–output gate* (where n, m are positive integers) is a special–purpose *computer* schematized as a device able to compute (Boolean) *logical functions* $G : \{0,1\}^n \to \{0,1\}^m$.

Reversible logic is a theoretical model of computation whose principal aim is to compute with zero *internal power dissipation*. Most of the times, computational models lack of *reversibility*; that is, one cannot in general deduce the input values of a gate from its output values. Lack of reversibility means that during the computation some information is lost. As shown by R. Landauer [24] (see also C.H. Bennett [25], [26] which can be found in [27]), a loss of information implies a loss of energy and therefore any computational model based on irreversible primitives is necessarily *informationally dissipative*. In this context, it is possible to prove that there is no information

energy dissipation by a classical gate iff the logical function computed by the gate is reversible (one-to-one and onto). Let us recall that any irreversible Boolean function $G : \{0,1\}^n \to \{0,1\}^m$ can always be transformed into a reversible function $G_r : \{0,1\}^{m+n} \to \{0,1\}^{m+n}$ assigning to the input pair $(\mathbf{x}, \mathbf{z}) \in \{0,1\}^n \times \{0,1\}^m$ the output pair $(\mathbf{x}, \mathbf{z} \oplus G(\mathbf{x})) \in \{0,1\}^n \times \{0,1\}^m$, where $\oplus$ is the extension to Boolean strings of the sum modulo 2 (i.e., the XOR 2–input/1–output Boolean gate. The original Boolean function can be recovered putting the second input $\mathbf{z}$ to $\mathbf{0}$: $(\mathbf{x}, \mathbf{0}) \to (\mathbf{x}, G(\mathbf{x}))$.

A system of *n-qubits*, or *quantum register* of n–length, is represented by a unit vector $|\Psi\rangle$ in the n–fold tensor product Hilbert space $\otimes^n \mathbb{C}^2$. A n–*configuration* is a unit vector $|x_1, ..., x_n\rangle \in \otimes^n \mathbb{C}^2$, quantum realization of the classical n–length string of bits $(x_1, ..., x_n) \in \{0,1\}^n$. Recall that $\mathcal{B}_c^{(n)} := \{|\mathbf{x}\rangle \in \otimes^n \mathbb{C}^2 : \mathbf{x} = (x_1, \ldots, x_n) \in \{0,1\}^n\}$ is an orthonormal basis of this space, called the *computational basis* for the n–quregisters.

Generally, the quantum realization of a n–input/n–output *reversible* Boolean gate $G : \{0,1\}^n \mapsto \{0,1\}^n$ is a transformation $T_G : \otimes^n \mathbb{C}^2 \to \otimes^n \mathbb{C}^2$ which, as a necessary condition, transforms quregisters of the computational basis $\mathcal{B}_c^{(n)}$ of $\otimes^n \mathbb{C}^2$ into quregisters of the same basis according to the condition:

$$|\mathbf{x}\rangle \mapsto T_G |\mathbf{x}\rangle = e^{i\omega(\mathbf{x})} |G(\mathbf{x})\rangle \tag{10}$$

where $\omega(\mathbf{x}) \in [0, 2\pi)$ is a given phase factor depending on the Boolean n length register $\mathbf{x} := (x_1, \ldots, x_n) \in \{0,1\}^n$. Since under the reversibility of the Boolean gate G, the condition (10) means in particular that it transforms an orthonormal basis of $\otimes^n \mathbb{C}^2$ into an orthonormal basis of the same space, the operator T_G turns out to be unitary or anti–unitary according to its linear or anti–linear extension to the whole Hilbert space. To be precise, let us denote by $|\Psi\rangle = \sum_{\mathbf{x} \in \{0,1\}^n} \langle \mathbf{x} |\Psi\rangle |\mathbf{x}\rangle$ the Fourier expansion of a generic vector Ψ from $\otimes^n \mathbb{C}^2$ with respect to the computational basis $\mathcal{B}_c^{(n)}$, then we have the two possible extensions of (10):

$$T_G^l |\Psi\rangle = \sum_{\mathbf{x} \in \{0,1\}^n} e^{i\omega(\mathbf{x})} \langle \mathbf{x} |\Psi\rangle |G(\mathbf{x})\rangle \qquad \text{Linear} \tag{11a}$$

$$T_G^a |\Psi\rangle = \sum_{\mathbf{x} \in \{0,1\}^n} e^{i\omega(\mathbf{x})} \langle \mathbf{x} |\Psi\rangle^* |G(\mathbf{x})\rangle \qquad \text{Anti–linear} \tag{11b}$$

On the set of density operators on $\otimes^n \mathbb{C}^2$, these quantum realizations of a Boolean gate G correspond to the intensity preserving operation generated by T_G expressed by $\Omega_G : \rho \mapsto \Omega_G(\rho) := T_G \circ \rho \circ T_G^{-1}$. In particular, whatever be the phase factor mapping $\omega : \mathbf{x} \to \omega(\mathbf{x})$, both these operators get a transformation of a pure state into a pure state according to

$$\rho_{|x_1, ..., x_n\rangle} \mapsto \Omega_G(\rho_{|x_1, ..., x_n\rangle}) = \rho_{|G(x_1, ..., x_n)\rangle}$$

As well known, in finite dimensional Hilbert spaces, both in the linear and in the anti–linear cases the above condition of being an operator Θ which transforms an orthonormal basis into another orthonormal basis can be assumed as the condition which defines unitary and anti–unitary operators

respectively. This condition is equivalent to the preservation of the norm (and so also of the distance – *isometry* condition): for every ψ, $\|\Theta\psi\| = \|\psi\|$. The two cases differ between them in a third equivalent formulation which in the linear case reads as: $\forall\psi, \varphi$, $\langle\Theta\psi|\Theta\varphi\rangle = \langle\psi|\varphi\rangle$ and in the anti–linear case as: $\forall\psi, \varphi$, $\langle\Theta\psi|\Theta\varphi\rangle = \langle\psi|\varphi\rangle^*$. This latter condition involving anti–linear operators can be formulated in the further equivalent way: "the operator Θ admits inverse Θ^{-1} and for any pair ψ, φ, $\langle\psi|\Theta^{-1}\varphi\rangle = \langle\Theta^{-1}\varphi|\psi\rangle^* = \langle\varphi|\Theta\psi\rangle$". The analogous formulation for the linear case is straightforward.

The role of anti–linear operators has been stressed by [28]: "it is becoming increasingly clear that anti–linear operators have an indispensable role in quantum field theory, so much so that the definition of the adjoint of such an operator can be found in a textbook on field theory by Itzykson and Zuber" [29]. To be precise, let us quote [30]: "The adjoint $\Theta^\dagger$ of an anti–linear operator Θ is determined by the relation $\langle\psi|\Theta^\dagger\varphi\rangle = \langle\varphi|\Theta\psi\rangle$ for all ψ, φ. Notice $\left(\Theta^\dagger\right)^\dagger = \Theta$. The standard rule $(AB)^\dagger = B^\dagger A^\dagger$ for linear operators remains valid if one or both operators are replaced by anti–linear ones. In particular, with a complex number a and anti–linear Θ one gets $\left(a\Theta\right)^\dagger = a\Theta^\dagger$, i.e., taking the adjoint $[\Theta \to \Theta^\dagger]$ is a linear procedure for anti–linear operators. [...] One calls Θ anti–linearly unitary or simply anti–unitary if $\Theta^\dagger = \Theta^{-1}$. Basic knowledge about anti–unitary operators is due to Wigner [31]".

The construction of the above operator (11b), in such a way that the computational basis is transformed into itself, means that the involved adjoint satisfies $(T_G^a)^\dagger = (T_G^a)^{-1}$, i.e., it is anti–unitary according to the just quoted definition.

From the physical point of view an anti–unitary operator can be considered an *internal symmetry* of the system. Indeed, for any state described by a non–zero vector ψ and any observable described by a linear bounded self–adjoint operator A let us denote by $\widehat{\psi} := \Theta\psi$ and $\widehat{A} := \Theta A \Theta^{-1}$ the transformed state and observable according to Θ. Then, the physical information on the system, enclosed into the real quantity $Exp\{\psi, A\} = \frac{\langle\psi|A\psi\rangle}{\|\psi\|^2}$, describing the expectation value of the observable A for the system prepared in ψ, is invariant with respect to the new description of the physical system produced by Θ. Indeed,

$$\frac{\langle\widehat{\psi}|\widehat{A}\widehat{\psi}\rangle}{\|\widehat{\psi}\|^2} = \frac{\langle\Theta\psi|\Theta A \psi\rangle}{\|\psi\|^2} = \frac{\langle\psi|A\psi\rangle^*}{\|\psi\|^2}$$

and so, from the self–adjoint property of A, $Exp\{\psi, A\} = Exp\{\widehat{\psi}, \widehat{A}\}$.

2.1 Unitary and anti–unitary quantum description of the Boolean IDENTITY gate

Let us apply these considerations to the simple Boolean *identity gate id* : $\{0, 1\} \mapsto \{0, 1\}$, characterized by the two trivial single bit transitions $0 \to$

$id(0) = 0$ and $1 \to id(1) = 1$. By the simplest choice of the phases $\omega(0) = \omega(1) = 0$, the (10) assumes in the present case the form of the two transitions:

$$T_{id} |0\rangle = |0\rangle \quad \text{and} \quad T_{id} |1\rangle = |1\rangle \tag{12}$$

and so the two formulations (11) applied to the generic vector $|\psi\rangle$ assume the forms:

$$T_{id}^l |\psi\rangle = \langle 0|\psi\rangle |id(0)\rangle + \langle 1|\psi\rangle |id(1)\rangle = |\psi\rangle$$
$$T_{id}^a |\psi\rangle = \langle 0|\psi\rangle^* |id(0)\rangle + \langle 1|\psi\rangle^* |id(1)\rangle$$

So the unitary realization is the standard linear identity operator on $\mathbb{C}^2$, $T_{id}^l = \mathbb{I}$. On the contrary, in the Heisenberg matrix representation of $\mathbb{C}^2$ with respect to the *canonical* computational basis $\mathcal{B}_c := \{|0\rangle, |1\rangle\}$ in which any vector $|\psi\rangle \in \mathbb{C}^2$ is represented by the "matrix" $\left(\begin{smallmatrix} \langle 0|\psi\rangle \\ \langle 1|\psi\rangle \end{smallmatrix}\right)$, the anti–unitary realization of the Boolean identity gate can be summarized by the transition:

$$\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \xrightarrow{T_{id}^a} \begin{pmatrix} c_0^* \\ c_1^* \end{pmatrix} \tag{13}$$

which, of course, satisfies the minimal conditions (12) and behaves as the identity on all the vectors of $\mathbb{C}^2$ with real components $c_0, c_1 \in \mathbb{R}$. Let us note that the anti–linear version T_{id}^a produces on the Poincaré sphere the transition $(P_x, P_y, P_z) \to (P_x, -P_y, P_z)$.

By the trivial extension of this complex conjugation anti–unitary operator to n–length qubits it is possible to express the following general link between the two unitary and unitary versions (11) of a classical reversible gate G given by the following relationship:

$$T_G^a = T_G^l \circ T_{id}^a = T_{id}^a \circ T_G^l \tag{14}$$

where the second commutativity identity follows from the fact that T_G^l transforms the computational basis into itself (reversibility of the classical gate G).

3 Unitary and anti-unitary quantum description of the classical Not gate

The classical NOT gate is a one-in/one-out Boolean gate $N : \{0,1\} \mapsto \{0,1\}$ defined by the transitions $0 \to 1$ and $1 \to 0$. Since this classical gate is characterized by a single line, its quantum description is mathematical realized on the single qubit Hilbert space $\mathbb{C}^2$. Hence, any quantum, either unitary or anti–unitary, realization T_N of the classical NOT gate on the Hilbert space $\mathbb{C}^2$ must satisfy the *minimal* conditions (10) translated to the present case:

$$T_N(|0\rangle) = e^{i\omega(0)} |1\rangle \quad \text{and} \quad T_N(|1\rangle) = e^{i\omega(1)} |0\rangle \tag{15}$$

These must be extended to the whole Hilbert space $\mathbb{C}^2$ according to one of the (11). In this way, the obtained transformation turns out to be unitary or anti-unitary according to the linear or anti-linear extension of T_N to any vector $|\psi\rangle \in \mathbb{C}^2$ such that $|\psi\rangle = \langle 0|\psi\rangle |0\rangle + \langle 1|\psi\rangle |1\rangle$.

3.1 Unitary extensions of the classical NOT gate

In this subsection we introduce a first unitary extension of the above minimal rules (15) describing the quantum behavior of the NOT classical gate, under the phase conditions $\omega(0) = \omega(1) = 0$:

$$T_N^l(|\psi\rangle) = \langle 1|\psi\rangle\,|0\rangle + \langle 0|\psi\rangle\,|1\rangle \tag{16}$$

whose (unitary) inverse is $(T_N^l)^{-1} = (T_N^l)^\dagger = T_N^l$, condition which expresses the self–reversibility of T_N^l. This unitary operator is nothing else than the Pauli spin matrix σ_x along the x direction.

For analogy with the forthcoming anti–unitary discussion we introduce now a second unitary extension $T_{N_1}^l : \mathbb{C}^2 \mapsto \mathbb{C}^2$ of the minimal conditions (15), under the phase conditions $\omega(0) = 0$ and $\omega(1) = \pi$:

$$T_{N_1}^l(|\psi\rangle) = \langle 1|\psi\rangle\,|0\rangle - \langle 0|\psi\rangle\,|1\rangle \tag{17}$$

described by the matrix

$$T_{N_1}^l = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y \tag{18}$$

Let us note that for any vector $|\psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle$ of $\mathbb{C}^2$, it is (adopting the standard Hilbert space notation $u_0 = |0\rangle$ and $u_1 = |1\rangle$, and not the Dirac one)

$$\langle\psi|T_{N_1}^l\psi\rangle = \langle c_0 u_0 + c_1 u_1 | c_1 u_0 - c_0 u_1\rangle = c_0^* c_1 - c_1^* c_0$$

which in general is different from 0. But in *all* the particular cases of real linear combinations $|\psi_r\rangle = r_0\,|0\rangle + r_1\,|1\rangle$, with $r_0, r_1 \in \mathbb{R}$, trivially one has that $\langle\psi_r|T_{N_1}^l\psi_r\rangle = 0$. We can conclude that in general the transformed of a $|\psi\rangle$ by $T_{N_1}^l$ is not orthogonal to this vector: $T_{N_1}^l\,|\psi\rangle \neq \big|\psi^\perp\big\rangle$. But if we consider the collection $\mathbb{C}_r^2 := \{|\psi\rangle = r_0\,|0\rangle + r_1\,|1\rangle : r_0, r_1 \in \mathbb{R}\}$, which is a real 2–dimensional linear space, then $\forall\,|\psi_r\rangle \in \mathbb{C}_r^2$, it is $T_{N_1}^l\,|\psi_r\rangle = \big|\psi_r^\perp\big\rangle$.

More generically, any unitary operator on $\mathbb{C}^2$ of the matrix form

$$T_{N_g} = \begin{pmatrix} 0 & e^{i\delta} \\ e^{i\gamma} & 0 \end{pmatrix} \quad \text{with inverse} \quad T_{N_g}^{-1} = T_{N_g}^\dagger = \begin{pmatrix} 0 & e^{-i\gamma} \\ e^{-i\delta} & 0 \end{pmatrix} \tag{19}$$

The first of which can also be formalized by the rule involving a generic superposition of the computational orthonormal basis as follows:

$$T_{N_g}(c_0\,|0\rangle + c_1\,|1\rangle) = e^{i\delta}\,c_1\,|0\rangle + e^{i\gamma}\,c_0\,|1\rangle$$

Trivially, also in this general case the transitions (15) are verified and this assures that any operator (19) is a good unitary realization of the classical Boolean NOT gate. Let us notice that the following holds:

$$\langle\psi|T_{N_g}\psi\rangle = \text{Re}(c_0^* c_1)\left(e^{i\delta} + e^{i\gamma}\right) + i\,\text{Im}(c_0^* c_1)\left(e^{i\delta} - e^{i\gamma}\right) \tag{20}$$

Thus,

1. in the particular case of $\delta = \gamma = 0$, corresponding to the unitary NOT–gate of (16), the (20) assumes the form $\langle \psi | T_N \psi \rangle = 2\,\mathrm{Re}(c_0^* c_1)$;
2. in the particular case of $\delta = 0$ and $\gamma = \pi$, corresponding to the unitary NOT$_1$–gate of (17), the (20) assumes the form $\langle \psi | T_{N_1} \psi \rangle = 2\,i\,\mathrm{Im}(c_0^* c_1)$, with the previously noticed property of complementation $\langle \psi | T_{N_1} \psi \rangle = 0$ in the real component case $c_0, c_1 \in \mathbb{R}$.

3.2 Anti-unitary extensions of the classical NOT gate.

In this subsection we analyze two *anti–unitary* extensions of the minimal conditions (15) along a parallelism with the just introduced linear extensions by an application of the general rule (11b). The first one is defined by the rule (compare with (16)):

$$T_N^a(|\psi\rangle) = \langle 1|\psi\rangle^* |0\rangle + \langle 0|\psi\rangle^* |1\rangle \tag{21}$$

The operator T_N^a is anti-unitary and self–reversible, with inverse $(T_N^a)^{-1} = (T_N^a)^\dagger = T_N^a$.

If for an application of the rule (11b) one takes inspiration from (17), we have the anti–unitary case defined by the law:

$$T_{N_1}^a(|\psi\rangle) = \langle 1|\psi\rangle^* |0\rangle - \langle 0|\psi\rangle^* |1\rangle \tag{22}$$

This operator $T_{N_1}^a : \mathbb{C}^2 \mapsto \mathbb{C}^2$ is just the one introduced in [4] and denoted by Θ in the introduction. Applying $T_{N_1}^a$ twice one obtains $-\mathbb{I}$ and so the inverse of $T_{N_1}^a$ is given by the anti–unitary operator $(T_{N_1}^a)^{-1} = -T_{N_1}^a$.

Differently from the linear case, for every $|\psi\rangle, |\varphi\rangle$ we have that

$$\left\langle \psi \mid T_{N_1}^a \varphi \right\rangle = \left\langle \varphi \mid (T_{N_1}^a)^{-1}\psi \right\rangle = \left\langle (T_{N_1}^a)^{-1}\psi \mid \varphi \right\rangle^* \tag{23}$$

As seen at the end of section 2, this is the condition which defines the adjoint of the anti–linear operator $T_{N_1}^a$ as $(T_{N_1}^a)^\dagger = (T_{N_1}^a)^{-1}$. In the particular case of $|\phi\rangle = |\psi\rangle$ one has that $\left\langle \psi \mid T_{N_1}^a \psi \right\rangle = \left\langle (T_{N_1}^a)^{-1}\psi \mid \psi \right\rangle$, which corresponds to the fact that $(T_{N_1}^a)^{-1}$ is the so–called *diagonal* adjoint of $T_{N_1}^a$. In particular $\left\langle \psi \mid T_{N_1}^a \psi \right\rangle = 0$ whatever be the vector $|\psi\rangle$. This result cannot be achieved by any of the other possible unitary and anti-unitary extensions of the classical NOT gates described before.

Making use of the conjugate anti–unitary operator T_{id}^a defined by (13) (and also of the unitary version of the NOT gate (16)), and according to the general relationship (14), we have that $T_{N_1}^a = T_{N_1}^l \circ T_{id}^a = i\sigma_y \circ T_{id}^a$, property which expresses "what can be called the *spin flip* transformation, [...]. For a pure state of a single qubit, the *spin flip* [...] is defined by

$$\left| \psi^\perp \right\rangle = i\sigma_y \left| \psi^* \right\rangle$$

where $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$ when it is expressed in a fixed basis such as $\{|\uparrow\rangle, |\downarrow\rangle\}$, and σ_y expressed in the same basis is the matrix

$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. For a spin-$\frac{1}{2}$ particle this is the standard time reversal operation and indeed reverses the direction of the spin" [32].

For any pure state (density operator) $\rho_{|\psi\rangle}$, it is

$$T^a_{N_1} \rho_{|\psi\rangle} (T^a_{N_1})^{-1} = \rho_{T^a_{N_1}|\psi\rangle}$$

corresponding to the fact that the von Neumann–Lüders operation (in the sense of [3]) generated by the anti–unitary operator $T^a_{N_1}$ transforms the pure state $\rho_{|\psi\rangle}$ into the "orthogonal" pure state $\rho_{T^a_{N_1}|\psi\rangle} = \rho_{|\psi^\perp\rangle}$.

4 Poincaré Sphere Considerations

In this section we analyze the unitary and anti-unitary operators introduced in the previous section as transformations on the Poincaré sphere. Let ρ be a density operator in the Hilbert space $\mathbb{C}^2$ uniquely represented in the form $\rho = \frac{1}{2}(\mathbb{I} + P_x\sigma_x + P_y\sigma_y + P_z\sigma_z) = \frac{1}{2}(\mathbb{I} + \underline{P}\cdot\underline{\sigma})$ under the condition $P_x^2 + P_y^2 + P_z^2 \le 1$. The correspondence $\rho \in \mathcal{TC}_1^+(\mathbb{C}^2) \longleftrightarrow \mathbf{P} = (P_x, P_y, P_z)$ is one-to-one and onto and so any density operator on $\mathbb{C}^2$ is univocally represented as a point of the Poincaré sphere of $\mathbb{R}^3$. Then, we have that:

1. $\rho \mapsto T^l_N \circ \rho \circ (T^l_N)^{-1}$ corresponds to the transformation $(P_x, P_y, P_z) \longrightarrow (P_x, -P_y, -P_z)$ in which the involved points are antipodes with respect to the x axis. In particular, any point on the zy plane of the Poincaré sphere $(0, P_y, P_z)$ is transformed into the *real* antipode $(0, -P_y, -P_z)$.
2. $\rho \mapsto T^l_{N_1} \circ \rho \circ (T^l_{N_1})^{-1}$ corresponds to the transformation $(P_x, P_y, P_z) \longrightarrow (-P_x, P_y, -P_z)$ in which the involved points are antipodes with respect to the y axis. Also in this case any point of the xz plane $(P_x, 0, P_z)$ is transformed by the unitary operator $T^l_{N_1}$ into its real antipodal $(-P_x, 0, -P_z)$.
3. $\rho \mapsto T^a_N \circ \rho \circ (T^a_N)^{-1}$ corresponds to transformation $(P_x, P_y, P_z) \longrightarrow (P_x, P_y, -P_z)$ in which the involved points are antipodes with respect to the xy plane.
4. $\rho \mapsto T^a_{N_1} \circ \rho \circ (T^a_{N_1})^{-1}$ corresponds to the transformation $(P_x, P_y, P_z) \longrightarrow (-P_x, -P_y, -P_z)$, such that *all* the involved pairs are antipodes of each other.

From point 4 we have that the anti–unitary BHW operator $T^a_{N_1}$ describes the gate which transforms any mixed state in another mixed state whose Poincaré representations are antipodal.

From the unitary point of view, the operator more similar to $T^a_{N_1}$ is $T^l_{N_1}$ which applied to a generic vector $|\vartheta, \varphi\rangle = \begin{pmatrix} e^{-i\frac{\varphi}{2}} \cos\frac{\vartheta}{2} \\ e^{i\frac{\varphi}{2}} \sin\frac{\vartheta}{2} \end{pmatrix}$ of $\mathbb{C}^2$ produces the transition:

$$|\vartheta, \varphi\rangle \xrightarrow{T^l_{N_1}} -|\vartheta + \pi, -\varphi\rangle = |\vartheta + \pi, -(\varphi + 2\pi)\rangle \qquad (24)$$

The outgoing vector $|\vartheta + \pi, -\varphi\rangle$ is the antipodal of the incoming one $|\vartheta, \varphi\rangle$, not with respect to the origin of the space $\mathbb{R}^3$ in which the Poincaré sphere is embedded, but with respect to its y axis.

The inner product $\langle \vartheta, \varphi | \vartheta + \pi, -\varphi \rangle = 2i \sin \varphi \cos \frac{\vartheta}{2} \sin \frac{\vartheta}{2}$ is trivially 0 (orthogonality) under the condition $\varphi = 0$, i.e., for any pure state of the form $|\vartheta, 0\rangle = \begin{pmatrix} \cos \frac{\vartheta}{2} \\ \sin \frac{\vartheta}{2} \end{pmatrix}$ i.e., with both the components real, whose Poincaré surface representation is on the xz plane. Under this condition the above transition (24) becomes

$$|\vartheta, 0\rangle \longrightarrow -|\vartheta + \pi, 0\rangle = |\vartheta + \pi, -2\pi\rangle$$

and so "if we relax the 'universality' condition, the U–NOT operation may become available: if we are promised that the elements of the density matrix (or the components of $|\varphi\rangle$) are *real*, the state lie in the $y = 0$ plane so that the inversion at the center is equivalent to a proper rotation by π around the y–axis". [6].

Setting $\vartheta = 2\alpha$, the vector $|\alpha\rangle = |2\alpha, 0\rangle$ describes the quantum (pure) state of light linear polarized along the direction α with respect to the reference axis $\mathbf{A}_1$ of the analyzer Nicol prism which constitute the preparation part of the device. In this interpretation the linear realization $T^l_{N_1}$ of the classical NOT gate performs an antipodal transformation of *all* possible pure states of linearly polarizations light.

These considerations can be extended to the case of states obtained as mixture of linear polarized pure states. Let $|\alpha\rangle$ and $|\alpha + \pi/2\rangle$ be the two quantum pure states of linear polarization about the mutually antipodal angles α and $\alpha + \pi/2$, for a fixed, but arbitrary α, with the operator representations $\rho_\alpha = |\alpha\rangle \langle \alpha|$ and $\rho_{\alpha+\pi/2} = |\alpha + \pi/2\rangle \langle \alpha + \pi/2|$. Let us make their generic convex combination $\rho_{\lambda,\alpha,\alpha+\pi/2} = \lambda \rho_\alpha + (1 - \lambda)\rho_{\alpha+\pi/2} = \frac{1}{2}\left[\mathbb{I} + (2\lambda - 1)\left(\sin(2\alpha)\, \sigma_x + \cos(2\alpha)\, \sigma_z \right) \right]$ with $0 \leq \lambda \leq 1$. Then, the associated Poincaré representation is the point $\left((2\lambda - 1) \sin(2\alpha), 0, (2\lambda - 1) \cos(2\alpha) \right)$ inside the unit xz circle of $\mathbb{R}^3$, whose antipodes has as corresponding density operator just $\rho_{\lambda,\alpha+\pi/2,\alpha} = \lambda\, \rho_{\alpha+\pi/2} + (1 - \lambda)\, \rho_\alpha = T^l_{N_1} \circ \rho_{\lambda,\alpha,\alpha+\pi/2} \circ (T^l_{N_1})^{-1}$.

5 Unitary and anti-unitary quantum description of the square root of the identity gate and of the square root of the Not gate

We will now consider two important *genuine quantum gates* that transform each element of the computational basis of $\mathbb{C}^2$ into qubits that are genuine superpositions of this basis: the *square root of the identity* and the *square root of the* NOT.

In this section, we consider in particular the following two operators on $\mathbb{C}^2$: the identity operator $\mathbb{I}$ and the linear version $T^l_{N_1}$ of the NOT gate with matrix representation (18). The identity operator is trivially positive since whatever be $\psi \neq \underline{0}$ it is $\langle \psi | \mathbb{I} \psi \rangle = \|\psi\|^2 \geq 0$, whose unique (positive) square root is, as expected, the identity operator itself $\sqrt{\mathbb{I}} = \mathbb{I}$. This is a particular application of the following general result of Functional Analysis.

Theorem. For every positive operator $T > \mathbb{O}$ it exists a unique positive operator $S \geq \mathbb{O}$ such that $S^2 = T$. In this case we write $S = \sqrt{T}$ and S is called the (positive) *square root* of T.

In order to extend this point of view to the case of unitary operators, one can take into account the following.

Definition. Given a unitary operator U we will say that a linear (resp., anti–linear) operator W is its unitary (resp., anti–unitary) *square root* iff W is unitary (resp., anti–unitary) and such that $W^2 = U$. In this case, for analogy, we will set $W = \sqrt{U}$.

The crucial point is that the existence of W does nor assure its uniqueness.

In the cases of our interest, the identity operator $\mathbb{I}$ and the linear version $T^l_{N_1}$ of the Boolean NOT gate, are both unitary and then it is possible to apply to them this definition of, in general non unique, (unitary) square root. For example, in the case of the identity operator we have seen that one possible square root is $\sqrt{\mathbb{I}} = \mathbb{I}$, which is positive and unitary. Moreover, two other (unitary) square roots of the identity $\mathbb{I}$ are the following Walsh–Hadamard (from now on simply Hadamard) operator and one of its variations, which are both self–adjoint and self–reversible but not positive:

$$H = H^\dagger = H^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \ \text{ and } \ H_1 = H_1^\dagger = (H_1)^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$$

Let us outline a generalization to the case of a *genuine* quantum gate (i.e., a gate which transforms at least an element of the computational basis into a superpositions of this basis) of the method (11) introduced in the case of *semi–classical* (i.e., quantum versions of classical Boolean) gates. For reasons of simplicity, we treat the case of the qubit Hilbert space $\mathbb{C}^2$ (the extension to the generic quregister case is straightforward). Fixed the computational basis $\mathcal{B}_c = \{|0\rangle, |1\rangle\}$ of $\mathbb{C}^2$ let us suppose to know the action of an operator U, linear or not, on the elements of this basis and formalized by the transformations:

$$U|0\rangle = a_0|0\rangle + a_1|1\rangle \tag{25a}$$
$$U|1\rangle = b_0|0\rangle + b_1|1\rangle \tag{25b}$$

where the outputs are superposition of the pure input qubits, but under the ortho–normality conditions:

$$\|U|0\rangle\|^2 = |a_0|^2 + |a_1|^2 = 1 \tag{26a}$$
$$\|U|1\rangle\|^2 = |b_0|^2 + |b_1|^2 = 1 \tag{26b}$$
$$\langle U|0\rangle \mid U|1\rangle \rangle = a_0^* b_0 + a_1^* b_1 = 0 \tag{26c}$$

Then, the generalization of (11) to a generic $|\psi\rangle = \langle 0|\psi\rangle |0\rangle + \langle 1|\psi\rangle |1\rangle$ is formalized as follows:

$$T^l_U |\psi\rangle = \langle 0|\psi\rangle \, U|0\rangle + \langle 1|\psi\rangle \, U|1\rangle \qquad \text{linear}$$
$$T^a_U |\psi\rangle = \langle 0|\psi\rangle^* U|0\rangle + \langle 1|\psi\rangle^* U|1\rangle \qquad \text{anti–linear}$$

that is

$$T^l_U |\psi\rangle = [a_0\langle 0|\psi\rangle + b_0\langle 1|\psi\rangle] \, |0\rangle + [a_1\langle 0|\psi\rangle + b_1\langle 1|\psi\rangle] \, |1\rangle \tag{27a}$$
$$T^a_U |\psi\rangle = [a_0\langle 0|\psi\rangle^* + b_0\langle 1|\psi\rangle^*] \, |0\rangle + [a_1\langle 0|\psi\rangle^* + b_1\langle 1|\psi\rangle^*] \, |1\rangle \tag{27b}$$

The above ortho–normality conditions (26) assure that both these operators transform an orthonormal basis into an orthonormal basis, and so they define a unitary and an anti–unitary operator, respectively. Moreover, these two unitary and anti–unitary versions are linked by an extension of the first relationship (14) furnished by the complex conjugation anti–unitary operator:

$$T_U^a = T_U^l \circ T_{id}^a \tag{28}$$

But differently from the second identity of (14), and taking into account the (25), we have that for an arbitrary $|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle$

$$T_U^l(T_{id}^a(c_0 |0\rangle + c_1 |1\rangle)) = c_0^*(a_0 + a_1) |0\rangle + c_1^*(b_0 + b_1) |1\rangle \tag{29a}$$

$$T_{id}^a(T_U^l(c_0 |0\rangle + c_1 |1\rangle)) = c_0^*(a_0^* + a_1^*) |0\rangle + c_1^*(b_0^* + b_1^*) |1\rangle \tag{29b}$$

Of course, if the coefficients involved in the equations (25) are all real, then we have that $T_U^l \circ T_{id}^a = T_{id}^a \circ T_U^l$, i.e., the involved extension commutes with the complex conjugation anti–unitary operator.

Moreover, since the involved coefficients are real, the two equations (29) are identical corresponding to the fact that

In particular, we apply the methods to the peculiar version of (25) for the case of the square root of the identity gate, formalized as

$$\sqrt{id} |0\rangle = \frac{1}{\sqrt{2}} \big[|0\rangle + |1\rangle \big] \tag{30a}$$

$$\sqrt{id} |1\rangle = \frac{1}{\sqrt{2}} \big[|0\rangle - |1\rangle \big] \tag{30b}$$

and for the case of the square root of the Not gate, formalized as

$$\sqrt{N_1} |0\rangle = \frac{1}{\sqrt{2}} \big[|0\rangle + |1\rangle \big] \tag{31a}$$

$$\sqrt{N_1} |1\rangle = \frac{1}{\sqrt{2}} \big[-|0\rangle + |1\rangle \big] \tag{31b}$$

Note that both these cases satisfies the ortho–normal conditions (26) which assure that the corresponding whole operators constructed according to the rules (27a) and (27b) are, respectively, unitary and anti–unitary. Note that all the involved coefficients are real, and so their extensions commute with the complex conjugation operator.

5.1 The unitary and anti–unitary versions of the square root of the identity gate

Making use of the (27a), the linear formulation of the above rules (30) describing the square root of the identity gate leads to the operator expressed by the law:

$$T_{\sqrt{id}}^l(|\psi\rangle) = \frac{1}{\sqrt{2}} [(\langle 0|\psi\rangle + \langle 1|\psi\rangle) |0\rangle + (\langle 0|\psi\rangle - \langle 1|\psi\rangle) |1\rangle] \tag{32}$$

This operator is unitary and self–reversible, i.e., $(T^l_{\sqrt{id}})^{-1} = (T^l_{\sqrt{id}})^\dagger = T^l_{\sqrt{id}}$, and its matrix representation with respect to the canonical computational basis is described by the Hadamard gate H

This unitary matrix acts on the generic vector $|\psi\rangle$ according to

$$T^l_{\sqrt{id}}|\psi\rangle = \frac{1}{\sqrt{2}}\big[\sigma_x|\psi\rangle + \sigma_z|\psi\rangle\big] \tag{33}$$

and it describes a self–reversible quantum gate, which is nothing else than the normalized sum of the Pauli spin–1/2 matrixes along the x and z directions. On the Poincaré sphere it produces the transition $(P_x, P_y, P_z) \to (P_z, -P_y, P_x)$.

On the other hand, the extension of the rules (30) expressed by the law (27b) leads to the anti–unitary operator

$$T^a_{\sqrt{id}}(|\psi\rangle) := \frac{1}{\sqrt{2}}[(\langle 0|\psi\rangle^* + \langle 1|\psi\rangle^*)\,|0\rangle + (\langle 0|\psi\rangle^* - \langle 1|\psi\rangle^*)\,|1\rangle] \tag{34}$$

This operator is again self–reversible $(T^a_{\sqrt{id}})^{-1} = T^a_{\sqrt{id}}$ and it produces the transition $(P_x, P_y, P_z) \to (P_z, P_y, P_x)$ on the Poincaré sphere.

Moreover, with respect to the generic vector $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$, the orthogonal (up to a phase factor) of the vector $\sigma_z|\psi\rangle = c_0|0\rangle - c_1|1\rangle$ is the vector $(\sigma_z|\psi\rangle)^\perp = -c_1^*|0\rangle - c_0^*|1\rangle$ and the orthogonal of the vector $\sigma_x|\psi\rangle = c_1|0\rangle + c_0|1\rangle$ is the vector $(\sigma_x|\psi\rangle)^\perp = c_0^*|0\rangle - c_1^*|1\rangle$. So the above (34), whatever be the incoming qubit $|\psi\rangle$, can be written as

$$T^a_{\sqrt{id}}|\psi\rangle = \frac{1}{\sqrt{2}}\big[(\sigma_x|\psi\rangle)^\perp - (\sigma_z|\psi\rangle)^\perp\big] \tag{35}$$

from which it follows that this operator can be expressed in term (besides others) of the anti–unitary universal NOT as follows

$$T^a_{\sqrt{id}} = \frac{1}{\sqrt{2}}\,T^a_{N_1}\big(\sigma_x - \sigma_z\big) \tag{36}$$

Thus, the anti–unitary operator $T^a_{\sqrt{id}}$ describes the transformation which satisfies the *condition* to take an *arbitrary* (unknown) qubit and to transform it into an equally superposition of two suitable qubits. Note that if the Poincaré representation of the pure state $|\psi\rangle$ is the triple (P_x, P_y, P_z), then the representation of the above pure state $\sigma_x|\psi\rangle$ (resp., $\sigma_z|\psi\rangle$) is the triple $(P_x, -P_y, -P_z)$ (resp., $(-P_x, -P_y, P_z)$), i.e., the antipodal with respect to the x (resp., z) axis of the representation of $|\psi\rangle$. Of course, the representation of the pure state $(\sigma_x|\psi\rangle)^\perp$ (resp., $(\sigma_z|\psi\rangle)^\perp$) is the triple $(-P_x, P_y, P_z)$ (resp., $(P_x, P_y, -P_z)$).

5.2 The non–linear version of the square root of the identity gate.

Taking inspiration from a comparison of the equations (17) and (22), one can suggest the rule that the passage from the linear case to the anti–linear one can be performed by the transformations $\langle 1|\psi\rangle\,|0\rangle \to \langle 1|\psi\rangle^*\,|0\rangle$ and $\langle 0|\psi\rangle\,|1\rangle \to \langle 0|\psi\rangle^*\,|1\rangle$. If we apply this heuristic rule to the (32) we get the operator defined by the law:

$$T^{nl}_{\sqrt{id}}(|\psi\rangle) := \frac{1}{\sqrt{2}}\left[\left(\langle 0|\psi\rangle + \langle 1|\psi\rangle^*\right)|0\rangle + \left(\langle 0|\psi\rangle^* - \langle 1|\psi\rangle\right)|1\rangle\right] \qquad (37)$$

Trivially, this operator is additive, but from

$$T^{nl}_{\sqrt{id}}(\alpha\,|\psi\rangle) = T^{nl}_{\sqrt{id}}\begin{pmatrix}\alpha\,c_0\\\alpha\,c_1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}\alpha\,c_0 + \alpha^*\,c_1{}^*\\-\alpha\,c_1 + \alpha^*\,c_0{}^*\end{pmatrix}$$

we immediately get that it is neither homogeneous, nor anti–homogeneous, nor absolutely homogeneous (but it is "real" homogeneous in the sense that $T^{nl}_{\sqrt{id}}(r\,|\psi\rangle) = r\,T^{nl}_{\sqrt{id}}\,|\psi\rangle$ for any real number $r \in \mathbb{R}$). In other words, we have to do with an additive, neither linear nor anti–linear operator $T^{nl}_{\sqrt{id}}$, which is self–reversible, $(T^{nl}_{\sqrt{id}})^{-1} = T^{nl}_{\sqrt{id}}$, preserves the "diagonal" inner product $\langle T^{nl}_{\sqrt{id}}\psi \mid T^{nl}_{\sqrt{id}}\psi\rangle = \langle\psi|\psi\rangle$ (and so the norm and the distance), whereas in general $\langle T^{nl}_{\sqrt{id}}\psi \mid T^{nl}_{\sqrt{id}}\varphi\rangle \neq \langle\psi|\varphi\rangle$ or $\langle T^{nl}_{\sqrt{id}}\psi \mid T^{nl}_{\sqrt{id}}\varphi\rangle \neq \langle\psi|\varphi\rangle^*$.

Moreover, with respect to the generic vector $|\psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle$, the orthogonal (up to a phase factor) of the vector $\sigma_z\,|\psi\rangle = c_0\,|0\rangle - c_1\,|1\rangle$ is the vector $(\sigma_z\,|\psi\rangle)^\perp = -c_1^*\,|0\rangle - c_0^*\,|1\rangle$ and so the above (37), whatever be the incoming qubit $|\psi\rangle$, can be written as

$$T^{nl}_{\sqrt{id}}\,|\psi\rangle = \frac{1}{\sqrt{2}}\left[\,\sigma_z\,|\psi\rangle - (\sigma_z\,|\psi\rangle)^\perp\right] \qquad (38)$$

In particular, this operator can be expressed in term of unitary and anti–unitary operators (besides others, of the anti–unitary universal NOT) as follows

$$T^{nl}_{\sqrt{id}} = \frac{1}{\sqrt{2}}\left(\mathbb{I} - T^a_{N_1}\right)\sigma_z$$

Thus, the non–linear operator $T^{nl}_{\sqrt{id}}$ describes the transformation which satisfies the *condition* to take an *arbitrary* (unknown) qubit and to transform it into an equally superposition of a suitable qubit and its orthogonal.

5.3 Unitary, anti–unitary, and non–linear versions of the square root of the Not gate.

Finally, we introduce the unitary version of the above conditions (31) describing the square root of the NOT gate.

$$T^l_{\sqrt{N_1}}(|\psi\rangle) = \frac{1}{\sqrt{2}}\left[\left(\langle 0|\psi\rangle + \langle 1|\psi\rangle\right)|0\rangle + \left(-\langle 0|\psi\rangle + \langle 1|\psi\rangle\right)|1\rangle\right]$$

On the Poincaré sphere it produces the transition $(P_x, P_y, P_z) \to (-P_z, P_y, P_x)$.

In the anti–linear case we have the operator defined by the law:

$$T^a_{\sqrt{N_1}}(|\psi\rangle) = \frac{1}{\sqrt{2}}\big[(\langle 0|\psi\rangle^* + \langle 1|\psi\rangle^*)\,|0\rangle + (-\langle 0|\psi\rangle^* + \langle 1|\psi\rangle^*)\,|1\rangle\big]$$

which according to (28) is obtained by the composition $T^a_{\sqrt{N_1}} = T^l_{\sqrt{N_1}} \circ T^a_{id}$. Let us note that, as pointed out at the discussion of the equation (31), since all the involved coefficients are real we have also that $T^a_{\sqrt{N_1}} = T^a_{id} \circ T^l_{\sqrt{N_1}}$. Hence, $T^a_{\sqrt{N_1}} \circ T^a_{\sqrt{N_1}} = T^l_{\sqrt{N_1}} \circ T^a_{id} \circ T^a_{id} \circ T^l_{\sqrt{N_1}} = T^l_{N_1}$.

Let us note that the anti–linear version $T^a_{\sqrt{N_1}}$ produces on the Poincaré sphere the transition $(P_x, P_y, P_z) \to (-P_z, -P_y, P_x)$.

Now, if one wants to describe a possible square root of the BHW anti–unitary operator (22), i.e., some operator W such that $W \circ W = T^a_{N_1}$, then such an operator cannot be either unitary or anti–unitary. Thus, it is necessary to seek inside non–linear operators. Making use of the heuristic procedure outlined above, we have the expected non–linear (only additive) operator defined by the law:

$$T^{nl}_{\sqrt{N_1}}(|\psi\rangle) = \frac{1}{\sqrt{2}}\big[(\langle 0|\psi\rangle + \langle 1|\psi\rangle^*)\,|0\rangle + (-\langle 0|\psi\rangle^* + \langle 1|\psi\rangle)\,|1\rangle\big]$$

This result, whatever be the qubit $|\psi\rangle$, with corresponding orthogonal $|\psi\rangle^\perp$, can be written as the following sum of a linear and an anti–linear operator:

$$T^{nl}_{\sqrt{N_1}}\,|\psi\rangle = \frac{1}{\sqrt{2}}\big[\,|\psi\rangle + |\psi\rangle^\perp\,\big] \tag{39}$$

Thus, the non–linear operator $T^{nl}_{\sqrt{N_1}}$ describes the transformation which satisfies the *universal condition* to take an *arbitrary* (unknown) qubit and to transform it into an equally superposition of the same qubit and the qubit orthogonal to it. This operator can be expressed in pure operator notation as

$$T^{nl}_{\sqrt{N_1}} = \frac{1}{\sqrt{2}}\big(\mathbb{I} + T^a_{N_1}\big)$$

6 Conclusions

In this paper we concentrate on one of the essential features of quantum information: the possibility of complementing it and we have seen that if from a classical point of view this corresponds to the simple transformations $0 \mapsto 1$, $1 \mapsto 0$, when the information is encoded in the generic state $|\psi\rangle$ of a quantum system the process of complementing a qubit $|\psi\rangle \mapsto |\psi^\perp\rangle$ is generally *impossible* by a *unique* unitary operation, where complementing means flipping a qubit on the Poincaré sphere. The problem can be traced back to the difference between classical and quantum ignorance, it touches on the very nature of the quantum state.

Since the manipulations on qubits have to be performed by unitary operations, the linearity of quantum theory seems to forbid complementing an unknown state. The process of complementing a qubit can be done *perfectly*, more precisely with fidelity 1, if and only if a basis to which $|\psi\rangle$ belongs is *known*: when the qubits are in preferred computational basis states the unitary operator $T_{N_1}^l$ realizes the quantum computational NOT gate *perfectly*, but it is not a *universal* one.

On the other side, the BHW operator $T_{N_1}^a$ represents an anti-unitary quantum NOT that is universal in a very strong sense: it takes any arbitrary unknown qubit $|\psi\rangle$ and transforms it *perfectly* into its orthogonal $|\psi^\perp\rangle$. This is a very desirable property, but if we ask for the universality condition then automatically we lose the possibility to realize a quantum not gate: $T_{N_1}^a$ is not completely positive. In this last case a possible solution comes from the quantum not gate introduced by Buzek-Hillery-Werner in [4] that *approximates* the anti-unitary transformation $T_{N_1}^a$ on the Hilbert space $\mathbb{C}^2$ by a unitary transformation on a larger Hilbert space such that it produces a complement of an arbitrary qubit $|\psi\rangle$ with fidelity $\frac{2}{3}$.

We suggest that the above analysis introduces two *complementary ways to describe the process to complement the information* encoded in a two level quantum system: unitary and anti-unitary one.

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