UNITARY AND ANTI-UNITARY QUANTUM DESCRIPTION OF THE CLASSICAL NOT GATE

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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 $0 \rightarrow 1$ and $1 \rightarrow 0$ (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). 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 superpositions: the square root of the identity and the square root of the negation.

Keywords: Quantum gates

1 Introduction

Recently a certain number of contributions \cite{1, 2, 3, 4, 5} has been published about the quantum version of the classical NOT gate as suitable operator on quantum realizations $|0\rangle$ and $|1\rangle$ of the classical bit 0 and 1 under the (minimal) condition of performing the two transformations $|0\rangle \rightarrow |1\rangle$ and $|1\rangle \rightarrow |0\rangle$ (the bit flipping condition). In literature (see for instance \cite{6, 7}) one can find some contributions according to which this quantum NOT gate can be mathematically realized as a unitary operator acting on the Hilbert space $\mathbb{C}^2$ describing spin 1/2 particles.
(for instance, electrons). To be precise, let \( \vec{u} = (u_x, u_y, u_z) \) be a fixed vector on the unit surface \( S_1(\mathbb{R}^3) \) (radius one surface of Euclidean space \( \mathbb{R}^3 \), centered in the zero vector), with polar representation \( \vec{u} = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta) \equiv (\vartheta, \varphi) \), and let us consider the orthonormal basis of \( \mathbb{C}^2 \)

\[
|\uparrow\vec{u}\rangle = \begin{pmatrix} e^{-i\varphi} \cos \frac{\vartheta}{2} \\ e^{i\varphi} \sin \frac{\vartheta}{2} \end{pmatrix} \quad |\downarrow\vec{u}\rangle = \begin{pmatrix} -e^{-i\varphi} \sin \frac{\vartheta}{2} \\ e^{i\varphi} \cos \frac{\vartheta}{2} \end{pmatrix}
\]

(1)

These are eigenvectors corresponding respectively to the eigenvalues +1 and −1 of the spin 1/2 observable along the \( \vec{u} \) direction

\[
\sigma_{\vec{u}} = \sigma(\vartheta, \varphi) = u_x \sigma_x + u_y \sigma_y + u_z \sigma_z = \begin{pmatrix} \cos \vartheta & e^{-i\varphi} \sin \vartheta \\ e^{i\varphi} \sin \vartheta & -\cos \vartheta \end{pmatrix}
\]

Let us stress that if one underlines the “angle dependence” of the first eigenvector, denoting this vector also as \( |\vartheta, \varphi\rangle := |\uparrow\vec{u}\rangle \) then trivially

\[
|\downarrow\vec{u}\rangle = \begin{pmatrix} -e^{-i\varphi} \sin \frac{\vartheta}{2} \\ e^{i\varphi} \cos \frac{\vartheta}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\varphi} \cos \frac{\vartheta + \pi}{2} \\ e^{i\varphi} \sin \frac{\vartheta + \pi}{2} \end{pmatrix} = |\vartheta + \pi, \varphi\rangle
\]

i.e., in the unit surface of \( \mathbb{R}^3 \) the involved unit vector is \( (\vartheta + \pi, \varphi) \equiv -\vec{u} \), the “antipodal” of the original unit vector \( \vec{u} \). Thus, as to the 1/2 spin interpretation we have that \( |\downarrow\vec{u}\rangle = \ket{\uparrow \vec{u}} \), the spin down eigenvector along \( \vec{u} \) coincides with the spin up eigenvector along its antipodal \( -\vec{u} \).

In this context, the quantum realization of the classical NOT gate is given by the unitary operator depending from the polar angles \( \vartheta, \varphi \):

\[
N(\vartheta, \varphi) := \begin{pmatrix} e^{i\varphi} & e^{-i\varphi} \\ e^{-i\varphi} (\cos^2 \frac{\vartheta}{2} - \sin^2 \frac{\vartheta}{2}) & e^{i\varphi} \sin \vartheta \end{pmatrix} = \begin{pmatrix} -\sin \vartheta & e^{-i\varphi} \cos \vartheta \\ e^{i\varphi} \cos \vartheta & \sin \vartheta \end{pmatrix}
\]

(2)

Indeed, if one set \( |0\rangle = |\uparrow\vec{u}\rangle \) and \( |1\rangle = |\downarrow\vec{u}\rangle \), then this operator realizes the transitions required to the quantum NOT gate. This is the answer of the following requirement:

- Given a fixed direction \( \vec{u} \in S_1(\mathbb{R}^3) \), there exists an operator (depending from \( \vec{u} \)) which performs the transformation of the unit vector \( |\uparrow\vec{u}\rangle = |\vartheta, \varphi\rangle \in \mathbb{C}^2 \) into its “antipodal” unit vector \( |\downarrow\vec{u}\rangle = |\vartheta + \pi, \varphi\rangle \in \mathbb{C}^2 \), and vice versa.

The unitary operator \( N \) is the required solution, since it transforms the “spin up” eigenvector along the direction \( \vec{u} \) in the opposite “spin down” along the same direction (or “spin up” along the opposite direction \( -\vec{u} \)). For this reason this unitary operator is said to be the mathematical realization of the logical NOT gate. Of course, it is not required (and in general this operator does not make) the same transformation from \( |\uparrow\vec{w}\rangle \) to \( |\downarrow\vec{w}\rangle \) in the case of a generic direction \( \vec{w} \neq \vec{u} \) from the unit sphere \( S_1(\mathbb{R}^3) \) of \( \mathbb{R}^3 \).

A totally different problem is to ask,

- whether it is possible to construct a unique operator which transforms the eigenvector \( |\uparrow\vec{u}\rangle = |\vartheta, \varphi\rangle \in \mathbb{C}^2 \) along any arbitrary direction \( \vec{u} \in S_1(\mathbb{R}^3) \) in the eigenvector \( |\downarrow\vec{u}\rangle = |\vartheta + \pi, \varphi\rangle \in \mathbb{C}^2 \) along the antipodal direction \( -\vec{u} \), and vice versa.
This is a quite different situation with respect to the previously discussed one. Indeed, in the first case the statement is of the form “for any (\(\forall\)) fixed direction, there exists (\(\exists\)) an operator such that (\(\ldots\))”, whereas in the second case we have to do with a statement of the form “there exist (\(\exists\)) an operator, such that for every (\(\forall\)) direction (\(\ldots\))”. In the context of unitary operators the latter question has a negative answer; conversely, a positive answer to this problem has been given in [1] by an anti–unitary operator. Thus, operators of this kind will be called mathematical representations of the quantum universal \textit{Not} gate (U–\textit{Not}), differently from the previous case of the simple \textit{logical Not} gate (L–\textit{Not}) in which one \textit{fixes} a particular direction \(\vec{u} \in S_1(\mathbb{R}^3)\) to give the quantum description of the classical bit 0 and 1 (thus, determined once for all) and then constructs a unitary operator which performs the required transformations of the classical \textit{Not} gate.

The difference between these two points of view is very important. Quoting from [1] “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 \textit{Not} gate. \textit{Complementing a qubit} (i.e., inverting the state of the spin–1/2 particles), however is another matter. The complement of a state \(|\Psi\rangle\) [our \(|\uparrow\rangle\) of Eq. (1)] is the state \(|\Psi^\perp\rangle\) [our \(|\downarrow\rangle\)] that is orthogonal to it.” If “complementing” a qubit means the choice of a state and give an operator which transforms it into its orthogonal, then this is done by the unitary operator (2), and this trivially corresponds to the quantum realization of the logical \textit{Not} gate. So “\textit{complementing a qubit}” is not a problem from this point of view. But if “the question we want to address is: Is it possible to build a device that will take an \textit{arbitrary} (unknown) qubit and transform it into the qubit orthogonal to it?” [1], then this is a totally different problem.

The aim of this paper is to show that operators of the kind (2) actually stay in an intermediate position between the two discussed above. Of course, they are not descriptions of a universal \textit{Not} gate, but they “complement” a lot of orthogonal pairs of states in addition to the pair described in Eq. (1). This means that if the complementation requirement is linked to some theoretical or practical necessity, than, contrary to the non physical anti–unitary realization, there is a unitary realization of the \textit{Not} gate which performs complementation of a certain number of orthopairs. In other words, if the BHW gate gives a positive answer to the full complementing requirement, but with the drawback of being anti–unitary, the logical \textit{Not} gate has the positive aspect to be unitary, but with the drawback of performing only a partial, also if sufficiently great, number of complementations.

1.1 \textit{The quantum description of light polarization}

Let us recall that on the Hilbert space \(\mathbb{C}^2\) it is possible to describe also the polarization states of photons (spin 1 Boson particles). This is a situation which is physically different from the spin 1/2 particle environment. For instance, in the case of electrons the 1/2 spin detection can be performed by Stern–Gerlach apparatuses whereas the observation of photon polarization can be done by Nicol prism apparatuses. All this leads to make attention to distinguish between the spin electron case and the photon polarization one, avoiding to make dangerous mixing of “\textit{spin} 1/2 particles \textit{polarized} along a direction.” [2].

In order to clarify the photon polarization situation about the mathematical description of light polarization on the Hilbert space \(\mathbb{C}^2\), let us make a brief discussion first of all quoting Fano [8, p. 79]:
Light polarization is represented by a density matrix with two rows and columns, corresponding to two opposite polarizations, e.g., to linear polarizations indicated by orthogonal unit vectors \( \mathbf{A}_1 \) and \( \mathbf{A}_2[\equiv \mathbf{A}^\dagger_1] \). Because of mathematical analogy to the density matrix for the orientation of spin–\( \frac{1}{2} \) particles, the density matrix of light polarization can be represented in the form

\[
\rho = \frac{1}{2} \left( \mathbf{I} + P_x \sigma_x + P_y \sigma_y + P_z \sigma_z \right) = \frac{1}{2} \left( \mathbf{I} + \mathbf{P} \cdot \mathbf{\sigma} \right)
\]

but the indices \( x, y, \) and \( z \) no longer correspond to direction of physical spaces.

They relate to a mathematical representation of polarizations in a 3–dimensional space, called “Poincaré representation,” in which

1. the [positive] \( z \) axis corresponds to linear polarization along \( \mathbf{A}_1 \),
2. negative \( z \) to polarization along \( \mathbf{A}_2[\equiv \mathbf{A}^\dagger_1] \),
3. positive \( x \) to linear polarization at \( 45^\circ \) between \( \mathbf{A}_1 \) and \( \mathbf{A}_2 \) and
4. positive \( y \) to circular polarization rotating from \( \mathbf{A}_1 \) toward \( \mathbf{A}_2 \).

In the above formula involving the density operator \( \rho \) on the Hilbert space \( \mathbf{C}^2 \), the components \( P_x, P_y, \) and \( P_z \) are relative to its Fourier expansion with respect to the “Pauli” orthonormal basis \( \{ \frac{1}{2}\mathbb{I}, \frac{1}{2}\sigma_x, \frac{1}{2}\sigma_y, \frac{1}{2}\sigma_z \} \) of the Hilbert space \( \mathcal{L}(\mathbf{C}^2) \) of all linear operators on \( \mathbf{C}^2 \), equipped with the inner product \( (A|B) := \text{Tr}[A^\dagger \circ B] \). In particular, \( P_j = (\rho|\sigma_j) = \text{Tr}[\rho \sigma_j] \), for \( j = x, y, z \), are the mean values of the operators represented by the three Pauli matrices \( \sigma_x, \sigma_y, \) and \( \sigma_z \) under the condition \( P_x^2 + P_y^2 + P_z^2 \leq 1 \). The correspondence \( \rho \in \mathcal{T}\mathcal{C}_1^+(\mathbf{C}^2) \leftrightarrow \mathbf{P} = (P_x, P_y, P_z) \in B_1(\mathbf{R}^3) \) is one-to-one and onto and so any density operator on \( \mathbf{C}^2 \) is univocally represented as a point of the Poincaré sphere \( B_1(\mathbf{R}^3) \) of \( \mathbf{R}^3 \). Precisely, the density operator represents a pure state iff \( P_x^2 + P_y^2 + P_z^2 = 1 \) and so \( (P_x, P_y, P_z) \) is a point on the surface \( S_1(\mathbf{R}^3) \) of the Poincaré sphere, otherwise the density operator is a proper mixture represented by an inner point of the sphere. In particular, the density operators \( |\mathbf{u}\rangle \langle \mathbf{u}| \) and \( |\mathbf{u}\rangle \langle \mathbf{v}| \) corresponding to the unit vectors \( \mathbf{u} \) are represented as points of the Poincaré surface \( S_1(\mathbf{R}^3) \) whose polar representation is just given by the pair of angles \( (\vartheta, \varphi) \) and \( (\vartheta + \pi, \varphi) \) respectively (antipodal Poincaré representation).

The Fano interpretation as light polarization can be explained by a quantum description of a standard experiment on linear polarization of light, with respect to a fixed reference axis represented by the unit vector \( \mathbf{A}_1 \). Consider first the elementary case of light prepared by a Nicol prism (the polarizer) in a state of linear polarization forming an angle \( \alpha \) with respect to the axis \( \mathbf{A}_1 \); the analysis of this linear polarized light can be performed by another Nicol prism (the analyzer) whose direction of polarization is \( \mathbf{A}_1 \). Therefore, “\( \alpha \) is the angle between the direction of polarization of the incident light and the direction of polarization of the light that would be fully transmitted by the [analyzer] prism.” \([9, \text{p. 859}]\). Summarizing, the second analyzer prism is fixed in the direction \( \mathbf{A}_1 \) and the first polarizer prism is rotated to prepare states at different angles \( \alpha \) of linear polarization with respect to \( \mathbf{A}_1 \).

Consider the (unit) vector \( |\mathbf{u}| = 2\alpha, \varphi = 0) = (\frac{\cos \alpha}{\sin \alpha}) \in \mathbf{C}^2 \), simply written as \( |\alpha\rangle \) and corresponding to a particular case of \( \mathbf{u} \), whose representation in terms of a pure state density operator is
\[ \rho_\alpha = \frac{1}{2} \begin{bmatrix} 1 + \sin(2\alpha) & \sin(2\alpha) \\ \sin(2\alpha) & 1 - \sin(2\alpha) \end{bmatrix} = \begin{bmatrix} \cos^2 \alpha & \sin \alpha \cos \alpha \\ \sin \alpha \cos \alpha & \sin^2 \alpha \end{bmatrix} \tag{3} \]

The spectral resolution of the third Pauli matrix \( \sigma_z \) consists of the following two projectors:

\[ E_z(\downarrow) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad E_z(\uparrow\uparrow) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{4} \]

These projectors describe two quantum events whose probabilities with respect to the state \( \rho_\alpha \) are given by \( \text{Tr}[\rho_\alpha E_z(\downarrow)] = \cos^2 \alpha = \frac{1}{2}(1+\cos 2\alpha) \) and \( \text{Tr}[\rho_\alpha E_z(\uparrow\uparrow)] = \sin^2 \alpha = \text{Tr}[\rho_{\alpha+\pi/2} E_z(\downarrow)] \). The former result is the quantum mechanical description of the empirical Malus law for a beam of linearly polarized photons prepared by a polarizer, where \( \alpha \) is the angle between the direction of polarization of the incident light and the direction of polarization of the analyzer.

The density matrix \( \rho_\alpha \) describes the state of the linearly polarized light produced from the polarizer forming an angle \( \alpha \) with respect to the reference axis \( A_1 \); the projector \( E_z(\downarrow) \) (resp., \( E_z(\uparrow\uparrow) \)) describes the event “the light is fully transmitted by the analyzer along the direction \( A_1 \) (resp., \( A_1^\perp \))”.

The vector of the Poincaré sphere associated with the density operator (3) is \( \vec{P}(\alpha) = (\sin 2\alpha, 0, \cos 2\alpha) \). It is worth noting that the Poincaré representation of any pure state of linear polarization (of a generic angle \( \alpha \) with respect to the reference unit vector \( A_1 \)) is characterized by the condition \( P_y = 0 \), i.e., are points of the \( xz \)-plane on the sphere.

In particular, the pure state of linear polarization along \( A_1 \) corresponds to \( \alpha = 0 \) and is described by the density operator \( \rho_0 = \frac{1}{2}(I + \sigma_z) \) with representation \( \vec{P}(0) = (0, 0, 1) \). Analogously, the pure state of linear polarization along \( A_1^\perp \) corresponds to \( \alpha = \pi/2 \) and is described by the density operator \( \rho_{\pi/2} = \frac{1}{2}(I - \sigma_z) \) with representation \( \vec{P}(0) = (0, 0, -1) \). A generic convex combination \( \rho := \lambda \rho_0 + (1 - \lambda) \rho_{\pi/2} \) describes a mixture of linear polarization along \( A_1 \) and \( A_1^\perp \) with weights \( \lambda \) and \( 1 - \lambda \), where \( 0 \leq \lambda \leq 1 \). Condition \( \lambda > 1/2 \) (resp., \( \lambda < 1/2 \)) describes a mixing in which the polarization along \( A_1 \) (resp., \( A_1^\perp \)) is prevalent. Trivially, it turns out that \( \rho = \frac{1}{2}[(I + (2\lambda - 1)\sigma_z)] \) with representation \( \vec{P} = (0, 0, 2\lambda - 1) \) which stays on the \( z \) axis of the Poincaré sphere according to the points (1) and (2) of the above quoted Fano statement. Similarly, the pure states of linear polarizations at \( \pi/4 = 45^\circ \) and \( 3\pi/4 = 135^\circ \) have the density operators \( \rho_{\pi/4} = \frac{1}{2}(I + \sigma_x) \) and \( \rho_{3\pi/4} = \frac{1}{2}(I - \sigma_x) \), with corresponding representations \( \vec{P}(\pi/4) = (1, 0, 0) \) and \( \vec{P}(3\pi/4) = (-1, 0, 0) \) respectively. The mixing state of these two linear polarization states is \( \rho = \lambda \rho_{\pi/4} + (1 - \lambda) \rho_{3\pi/4} = \frac{1}{2}[(I + (2\lambda - 1)\sigma_x)] \), with associated representation \( \vec{P}(\rho) = (2\lambda - 1, 0, 0) \) which stays on the \( x \) axis. Also in this case the condition \( \lambda > 1/2 \) (resp., \( \lambda < 1/2 \)) describes a mixture in which the linear polarization along \( 45^\circ \) (resp., \( 135^\circ \)) is predominant with respect to the other one; moreover, the corresponding point in the Poincaré sphere stays on the positive (resp., negative) part of the \( x \) axis.

Let us consider now the orthonormal basis of \( \mathbf{C}^2 \) consisting of the two vectors

\[ |R(\vartheta)\rangle = \begin{pmatrix} -i \cos \vartheta \\ \sin \vartheta \end{pmatrix} \quad |L(\vartheta)\rangle = \begin{pmatrix} i \sin \vartheta \\ \cos \vartheta \end{pmatrix} \]
whose associated density matrices are respectively:

\[
\rho_{R(\vartheta)} = \frac{1}{2} \left[ I + \cos \vartheta \sigma_z - \sin \vartheta \sigma_y \right] = \frac{1}{2} \begin{pmatrix} 1 + \cos \vartheta & i \sin \vartheta \\ -i \sin \vartheta & 1 - \cos \vartheta \end{pmatrix}
\]

\[
\rho_{L(\vartheta)} = \frac{1}{2} \left[ I - \cos \vartheta \sigma_z + \sin \vartheta \sigma_y \right] = \frac{1}{2} \begin{pmatrix} 1 - \cos \vartheta & -i \sin \vartheta \\ i \sin \vartheta & 1 + \cos \vartheta \end{pmatrix}
\]

These two pure states describe right and left hand elliptical (complete) polarizations of light, parameterized by the angle \( \vartheta \). Right and left hand circular polarizations correspond to the angle \( \vartheta = \pi/2 \), whereas \( \mathbf{A}_1 \) and \( \mathbf{A}_{\perp 1} \) linear polarizations correspond to the angle \( \vartheta = 0 \). These latter cases can be considered degenerate form of elliptic polarization. The associated representative (diametrically opposed or antipodal) points on the Poincaré sphere are \( \vec{P}(R(\vartheta)) = (0, -\sin \vartheta, \cos \vartheta) \) and \( \vec{P}(L(\vartheta)) = (0, \sin \vartheta, -\cos \vartheta) \), respectively, i.e., points from the \( yz \)-plane of the Poincaré sphere.

This discussion about light polarization in quantum mechanics can be summarized by the following rules:

1. The two states \( \mathbf{1} \) of \( \mathbb{C}^2 \) are orthogonal between them and they Poincaré representation is given by antipodal points of the unit sphere of \( \mathbb{R}^3 \) (orthogonality on \( \mathbb{C}^2 \) corresponds to antipodal points on the unit sphere of \( \mathbb{R}^3 \)).

2. Linear polarization corresponds to the particular case of \( \vartheta = 2\alpha \) and \( \varphi = 0 \), whose Poincaré representations are on the \( xz \)-plane. In particular, the two orthogonal states

\[
|\downarrow\alpha\rangle = \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix} \quad \text{and} \quad |\leftrightarrow\alpha\rangle = \begin{pmatrix} -\sin \alpha \\ \cos \alpha \end{pmatrix} = |\downarrow\alpha + \pi/2\rangle
\]

describe two quantum states of linear polarization along two mutually orthogonal directions \( \alpha \) and \( \alpha + \pi/2 \) of the physical space respectively.

3. Elliptical polarization states are linked to the states of \( \mathbf{1} \) by the relationships \( |\vartheta, \pi/2\rangle = e^{i\pi/4} |R(\vartheta)\rangle \) and \( |\vartheta + \pi, \pi/2\rangle = e^{i\pi/4} |L(\vartheta)\rangle \), whose (antipodal) Poincaré representations are on the \( yz \)-plane.

In conclusion of this introduction, we hope to clarify the foundational aspects of the debate about the alternative unitary – anti-unitary dichotomy in describing from the quantum point of view the classical NOT gate, making a clear distinction about its use as a qubit transformation along a fixed direction (simple quantum NOT gate) profoundly different from the role of the universal quantum NOT gate, in which the qubit transformation is performed by the same gate along any possible direction.

2 Unitary and anti–unitary operators in axiomatic quantum mechanics on Hilbert spaces

In the standard unsharp axiomatic quantum mechanics based on a (complex, separable) Hilbert space \( \mathcal{H} \) states are mathematically described by positive trace class of trace 1 linear operators (whose collection will be denoted by \( \mathcal{T}_1^+(\mathcal{H}) \)), effects by positive \( \langle \psi \psi \rangle \in \mathcal{H} : \langle \psi | F \psi \rangle \geq 0 \) and absorbing \( \langle \psi \in \mathcal{H} : \langle \psi | F \psi \rangle \leq \| \psi \|^2 \) linear operators \( F \) (whose collection will be denoted by \( \mathcal{F}(\mathcal{H}) \)), and the Born probability rule by the mapping \( p: \mathcal{T}_1^+(\mathcal{H}) \times \mathcal{F} \rightarrow [0, 1] \) which
associates to any pair consisting of a state \( \rho \in \mathcal{T}(\mathcal{H}) \) and an effect \( F \in \mathcal{F} \) the probability \( p(\rho, F) := \text{Tr}(\rho F) \in [0,1] \).

Let us note that in the case of a pure state \( \rho[\psi] = |\psi\rangle \langle \psi| \) described by the ray of vectors 
\[ \rho[\psi] := \{ e^{i\theta} \psi \in \mathcal{H} : \theta \in [0,2\pi) \} \]
generated by the unit vector \( \psi \in \mathcal{H} \), the Born probability rule becomes \( p(\rho[\psi], F) = \langle \psi|F\psi \rangle \), which is invariant with respect to any choice of the unit representative of the state \( |\psi\rangle \). In this case we shall denote the Born probability simply by \( p(\psi, F) \). Moreover, in the sequel we will denote by \( \psi \approx \psi' \) the fact that these two unit vectors belong to the same ray.

Trivially, orthogonal projections are effect operators and in the particular case of the orthogonal projection \( P[\psi] = |\psi\rangle \langle \psi| \) generated by the unit vector \( \psi \), the Born probability with respect to any pure state \( \rho[\psi] \) is
\[
p(\rho[\psi], P[\psi]) = |\langle \phi|\psi \rangle|^2
\]
which is independent from the representative of the involved states, i.e., \( |\langle \phi|\psi \rangle|^2 = |\langle \phi'|\psi' \rangle|^2 \) whatever be \( \psi' \approx \psi \) and \( \phi' \approx \phi \). This suggest the introduction of the “inner product” of two rays \( \Phi := [\phi] \) and \( \Psi := [\psi] \) defined as
\[
\Phi \cdot \Psi = |\langle \phi|\psi \rangle|^2 \quad (\phi \in \Phi, \psi \in \Psi)
\] (5)
also called the transition probability from the pure state \( \Phi \) to the pure state \( \Psi \). Trivially, \( p(\rho[\phi], P[\psi]) = p(\rho[\psi], P[\phi]) \) and so the transition probability \( \Phi \rightarrow \Psi \) is equal to the transition probability \( \Psi \rightarrow \Phi \).

In this paper we are particularly interested to a comparison between unitary and anti–unitary quantum description of the well known classical Boolean NOT gate. To this end, let us now introduce two important results which illustrate the “parallel” role played both from unitary and anti–unitary operators in quantum mechanics.

### 2.1 Wigner’s theorem on symmetry operations

Let us now recall a well known Wigner’s theorem about symmetry operations \([10]\) (in the version proposed by Bargmann \([10]\)), which for the scope of the present paper is restricted to the case of symmetries internal to a fixed Hilbert space.

A symmetry operation \( T \) (called also invariance principle, or simply symmetry) internal to a Hilbert space \( \mathcal{H} \) is an onto correspondence which yields for each pure state \( \Phi = [\phi] \) of the Hilbert space \( \mathcal{H} \), another pure state \( \Phi' = [\phi'] \) of the same Hilbert space, such that all the transition probabilities are preserved. In terms of rays, \( T \) defines a mapping \( \Phi \mapsto \Phi' = T(\Phi) \) of rays onto rays such that
\[
\Phi'_1 \cdot \Phi'_2 = \Phi_1 \cdot \Phi_2 \quad \text{if} \quad \Phi'_1 = T(\Phi_1)
\] (6)
(Note that this condition of preservation of transition probabilities implies that the mapping \( T \) is one-to-one). In terms of representatives of states this condition can be expressed as follows:
\[
|\langle \phi'|\phi'_2 \rangle|^2 = |\langle \phi_1|\phi_2 \rangle|^2 \quad \text{if} \quad \phi_i \in \Phi_i \text{ and } \phi'_i \in \Phi'_i
\]
The Wigner’s theorem says that every such ray mapping \( T \) can be replaced by a vector mapping \( T' \) of \( \mathcal{H} \) which is either unitary or anti–unitary. Precisely, there exists a mapping

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$T : \mathcal{H} \mapsto \mathcal{H}$, either unitary or anti–unitary, such that $\phi \in \Phi$ implies $T(\phi) \in \mathcal{T}(\Phi)$. Trivially, putting together (\text{4}) with (\text{5}), this implies that

$$|(T(\phi_1)|T(\phi_2)|)^2 = |\phi_1|\phi_2|^2 \quad \text{if} \quad \phi_1 \in \Phi.$$ 

Adopting the Bargmann’s terminology, the operator $T$ is said to be compatible with $\mathcal{T}$, and $\mathcal{T}$ is said to be generated by (or an extension of) the mapping $T$. It is clear that any unitary or anti–unitary operator $T$ induces a symmetry $\mathcal{T}$ associating to any ray $|\phi\rangle$ the corresponding ray $T|\phi\rangle := |T(\phi)\rangle$. Wigner’s theorem asserts that any symmetry is generated only by operators of this kind.

As a last remark, if $T_1$ and $T_2$ are both unitary (resp., anti–unitary) and generate the same symmetry $\mathcal{T}$, then $T_2 = e^{i\theta}T_1$ if $\text{dim}(\mathcal{H}) \geq 2$. Hence, the operator $T$ of the Wigner’s theorem is uniquely determined up to a phase.

### 2.2 Intensity preserving operations on beam preparations

If in some physical applications it would be interesting to describe preparation, filtering and detection of beams with some intensities, following Mielnik [11], the mathematical description of preparations on the Hilbert space $\mathcal{H}$ could be realized by non–negative and trace class operators $\eta \in \mathcal{T}\mathcal{C}^+(\mathcal{H})$, whose trace is not necessarily equal to one: $\text{Tr}(\eta) \in \mathbb{R}_+$. This non–negative quantity is just assumed as the intensity of the beam prepared be $\eta$: $I(\eta) := \text{Tr}(\eta)$. A pure preparation is described by the one dimensional subspace $[[\psi]] = \{c\psi \in \mathcal{H} : c \in \mathbb{C}\}$ generated by the (non necessarily of norm one) vector $\psi \in \mathcal{H}$ and is represented by the operator $\eta_{[[\psi]]} = |\psi\rangle\langle\psi| \in \mathcal{T}\mathcal{C}^+(\mathcal{H})$. This pure preparation operator is invariant with respect to the choice of the representative vector from $[[\psi]]$ and its intensity is $I(\eta_{[[\psi]]}) = ||\psi||^2$.

Note that any preparation operator $\eta \in \mathcal{T}\mathcal{C}^+(\mathcal{H})$ generates a density operator by a standard normalization procedure $\rho_\eta := \frac{\eta_{[[\psi]]}}{\text{Tr}(\eta)}$. In particular the pure preparation operator $\eta_{[[\psi]]} = |\psi\rangle\langle\psi|$ generates the pure density operator $\rho_{\eta_{[[\psi]]}} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \rho_{|\psi\rangle/||\psi||}$.

Denoted by $V(\mathcal{H})$ the Banach space of self–adjoint trace class operators with the trace norm and by $V^+(\mathcal{H}) = \mathcal{T}\mathcal{C}^+(\mathcal{H})$ the cone of non–negative trace class operators (preparation operators), according to [12] an operations on $V(\mathcal{H})$ is a linear mapping $\Omega : V(\mathcal{H}) \to V(\mathcal{H})$ which is positive (i.e., $\Omega(\eta) \in V^+(\mathcal{H})$ for any preparation $\eta \in V^+(\mathcal{H})$) and absorbing (i.e., $0 \leq \text{Tr}(\Omega(\eta)) \leq \text{Tr}(\eta)$ for any preparation $\eta \in V^+(\mathcal{H})$). From a physical point of view, the positivity condition means that an operation $\Omega$ must transform an incoming preparation $\eta$ in an outgoing preparation $\Omega(\eta)$, filtering some effects on the systems which constitute the incoming beam. The filtering produces a decrease of the incoming beam intensity $I(\eta) = \text{Tr}(\eta)$ such that the outgoing beam intensity turns out to be $I(\Omega(\eta)) = \text{Tr}(\Omega(\eta))$. This corresponds to a probability of filtering expressed by the ratio $p_f(\eta, \Omega) := \frac{\text{Tr}(\Omega(\eta))}{\text{Tr}(\eta)}$ \in [0,1].

Hence, an operation describes a genuine filter if there exists at least a preparation $\eta_0$ such that $I(\Omega(\eta_0)) < I(\eta_0)$.

On the contrary there are operations which are intensity (also trace) preserving, i.e., such that for every preparation $\eta$ it is $I(\Omega(\eta)) = I(\eta)$. As to this class of operation, in [12] p. 25 one can find the following result.

Let $\Omega : V(\mathcal{H}) \to V(\mathcal{H})$ be an intensity preserving operation with positive inverse. Then
there exists a unitary or anti-unitary map $U$ on $\mathcal{H}$ such that for all $\eta \in V(\mathcal{H})$

$$\Omega(\eta) = U \circ \eta \circ U^{-1}$$

(7)

The operator $U$ is uniquely determined up to a constant of absolute value one.

3 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, \{\text{AND}, \text{NOT}\}. From a general point of view, a classical (Boolean) \textit{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 $G : \{0,1\}^n \rightarrow \{0,1\}^m$.

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 [13] (see also C.H. Bennett [14, 15] which can be found in [16]), 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 the information energy dissipation of a gate is 0 iff the logical function computed by the gate is reversible (one-to-one and onto). Let us recall that any irreversible Boolean function $G : \{0,1\}^n \rightarrow \{0,1\}^m$ can always be transformed into a reversible function $G_r : \{0,1\}^{m+n} \rightarrow \{0,1\}^{m+n}$ assigning to the input pair $(\vec{x}, \vec{z}) \in \{0,1\}^n \times \{0,1\}^m$ the output pair $(\vec{x}, \vec{z} \oplus G(\vec{x})) \in \{0,1\}^n \times \{0,1\}^m$, where $\oplus$ is the sum modulo 2 (XOR 2–input/1–output Boolean gate). The original Boolean function can be recovered putting the second input $\vec{z}$ to 0: $(\vec{x}, 0) \rightarrow (\vec{x}, G(\vec{x}))$.

In the theory of Quantum Computation and Quantum Information the information is elaborated and transmitted by two-level quantum systems, the qubits whose mathematical description is based on the two-dimensional complex Hilbert space $\mathbb{C}^2$. The unit vectors of the orthonormal basis $|\vec{e} \rangle$, in this context called the computational basis of $\mathbb{C}^2$, represent two states for a qubit that correspond two the Boolean states 0 and 1, denoted also by $\{0\} \cup \{1\}$ or simply by $\{0\} \cup \{1\}$ if no confusion is likely. But, unlike the bit, a qubit can be in a state other than $|0\rangle$ or $|1\rangle$, precisely in states which are superposition of these latter $|\psi\rangle = c_1|0\rangle + c_2|1\rangle$, where $c_1, c_2$ are complex number such that $|c_1|^2 + |c_2|^2 = 1$.

A system of \textit{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 $|x_1, \ldots, x_n\rangle \in \otimes^n \mathbb{C}^2$, quantum realization of the classical $n$–length string of bits $(x_1, \ldots, x_n) \in \{0,1\}^n$. Recall that $\mathcal{B}_c := \{|\vec{x}\rangle \in \otimes^n \mathbb{C}^2 : \vec{x} = (x_1, \ldots, x_n) \in \{0,1\}^n\}$ is an orthonormal basis of this space, called the computational basis for the $n$–qregisters.

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

$$|\vec{x}\rangle \mapsto T_G |\vec{x}\rangle = e^{i\Theta(\vec{x})} |G(\vec{x})\rangle$$

(8)
where $\Theta(\vec{x}) \in [0, 2\pi)$ is a given phase factor depending from the Boolean $n$ length register \( \vec{x} := (x_1, \ldots, x_n) \in \{0, 1\}^n \). This transformation turns out to be a unitary or anti–unitary operator according to the linear or anti–linear extension of $T_G$ to the whole Hilbert space. To be precise, let us denote by $|\Psi\rangle = \sum_{\vec{x} \in \{0, 1\}^n} \langle \vec{x} | \Psi \rangle |\vec{x}\rangle$ the Fourier expansion with respect to computational basis $\mathcal{B}_c$ of any vector $\Psi$ from $\otimes^n \mathbb{C}^2$, then

$$
T_G |\Psi\rangle = \begin{cases} 
\sum_{\vec{x} \in \{0, 1\}^n} e^{i\Theta(\vec{x})} \langle \vec{x} | \Psi \rangle |G(\vec{x})\rangle & \text{Linear} \\
\sum_{\vec{x} \in \{0, 1\}^n} e^{i\Theta(\vec{x})} \langle \vec{x} | \Psi \rangle^* |G(\vec{x})\rangle & \text{Anti–linear}
\end{cases}
$$

(9)

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 \( \Theta \) 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 $\Theta : \vec{x} \to \Theta(\vec{x})$, \( \rho_{|x_1, \ldots, x_n} \mapsto \Omega_G(\rho) = \rho_{|G(x_1, \ldots, x_n)} \)

4 Unitary and anti-unitary quantum description of the classical NOT gate

The classical NOT gate is a one–in/on-out Boolean gate $N : \{0, 1\} \to \{0, 1\}$ 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 mathematically realized on the single qubit Hilbert space $\mathbb{C}^2$ (quantum register of length 1). From now on, and for the sake of simplicity since the general case can be treated in a straightforward way, we assume that the classical bits $\{0, 1\}$ are represented by the two unit vectors of the canonical orthonormal basis $\mathcal{B}_c := \{|0\rangle = |\frac{1}{\sqrt{2}}\rangle, |1\rangle = |\frac{1}{\sqrt{2}}\rangle\}$ of $\mathbb{C}^2$. 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 \( \Theta \) translated to the present case

$$
T_N(|0\rangle) = e^{i\Theta(0)} \text{ and } T_N(|1\rangle) = e^{i\Theta(1)}
$$

(10)

extended to the whole Hilbert space $\mathbb{C}^2$ following \( \Theta \). In this way, this 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 $|\psi\rangle = \langle 0 | \psi \rangle |0\rangle + \langle 1 | \psi \rangle |1\rangle$.

4.1 Linear extensions of the NOT gate.

In this subsection we introduce a first linear extension of the above minimal rules describing the quantum behavior of the NOT classical gate.

$$
T_N^l(|\psi\rangle) = \langle 0 | \psi \rangle |1\rangle + \langle 1 | \psi \rangle |0\rangle
$$

(11)

For $c_1 = \langle 0 | \psi \rangle$ and $c_2 = \langle 1 | \psi \rangle$, the operator $T_N^l : \mathbb{C}^2 \to \mathbb{C}^2$ produces the transformation

$$
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \to T_N^l \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_1 \end{pmatrix}
$$

(12)

that can be also expressed as $T_N^l(c_1 |0\rangle + c_2 |1\rangle) = c_2 |0\rangle + c_1 |1\rangle$. The operator $T_N^l$ is unitary with (unitary) inverse $(T_N^l)^{-1} = (T_N^l)^\dagger = T_N^l$ and is defined by the matrix

$$
T_N^l = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x
$$

(13)

This unitary operator describes in this way a self–reversible quantum gate, which is nothing else than the Pauli spin matrix along the $x$ direction.
4.1.1 Another linear extension.

For analogy with the forthcoming anti–linear discussion we introduce now a second linear extension of minimal conditions (10) according to:

\[ T_{N_1}^l(|\psi\rangle) = |1\rangle \langle 1| |0\rangle - |0\rangle \langle 0| |1\rangle \]  

(14)

The operator \( T_{N_1}^l : \mathbb{C}^2 \rightarrow \mathbb{C}^2 \) corresponds to transformation

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow \begin{pmatrix} c_2 \\ -c_1 \end{pmatrix}
\]

(15)

that can be also expressed as \( T_{N_1}^l (c_1 |0\rangle + c_2 |1\rangle) = c_2 |0\rangle - c_1 |1\rangle \) and is defined by the matrix

\[
T_{N_1}^l = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}
\]

(16)

whose inverse is the matrix \( (T_{N_1}^l)^{-1} = (T_{N_1}^l)^\dagger = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \).

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

\[
T_{N_g} = \begin{pmatrix} 0 & e^{i\delta} \\ e^{i\gamma} & 0 \end{pmatrix}
\]

with inverse \( T_{N_g}^\dagger = \begin{pmatrix} 0 & e^{-i\gamma} \\ e^{-i\delta} & 0 \end{pmatrix} \) (17)

produces the transition

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow T_{N_g} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} e^{i\delta} c_2 \\ -e^{i\gamma} c_1 \end{pmatrix}
\]

(18)

which can also be formalized by the rule involving a generic superposition of the canonical orthonormal basis

\[
T_{N_g} (c_1 |0\rangle + c_2 |1\rangle) = e^{i\delta} c_1 |1\rangle + e^{i\gamma} c_2 |0\rangle
\]

(19)

Trivially, also in this generic case the transitions (10) are verified and this assures that any operator (17) is a good unitary realization of the classical Boolean NOT gate. Let us notice that the following holds:

\[
\langle \psi | T_{N_g} | \psi \rangle = \text{Re}(c_1^* c_2) (e^{i\delta} + e^{i\gamma}) + \text{Im}(c_1^* c_2) (e^{i\delta} - e^{i\gamma})
\]

(20)

Thus,

1. in the particular case of \( \delta = \gamma = 0 \), corresponding to the unitary NOT–gate of (11), the (20) assumes the form \( \langle \psi | T_{N} | \psi \rangle = 2 \text{Re}(c_1^* c_2) \);  
2. in the particular case of \( \delta = 0 \) and \( \gamma = \pi \), corresponding to the unitary NOT\(_1\)–gate of (14), the (20) assumes the form \( \langle \psi | T_{N_1} | \psi \rangle = 2 i \text{Im}(c_1^* c_2) \).
4.2 Anti-linear extension of the classical Not gate.

In this subsection we analyze two anti-linear extensions of the minimal conditions \([\text{10]}\) along a parallelism with the just introduced linear extensions. The first one is defined by the rule (compare with \([\text{11]}\)):

\[
T^a_N(|\psi\rangle) = \langle 0|\psi\rangle^*|1\rangle + \langle 1|\psi\rangle^*|0\rangle
\]

The operator \(T^a_N : \mathbb{C}^2 \rightarrow \mathbb{C}^2\) produces the transition

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow T^a_N \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} c_2^* \\ c_1^* \end{pmatrix}
\]

that can be also expressed as \(T^a_N(c_1|0\rangle + c_2|1\rangle) = c_2^*|0\rangle + c_1^*|1\rangle\). \(T^a_N\) is anti-unitary with inverse \((T^a_N)^{-1} = (T^a_N)^\dagger = T^a_N\).

4.2.1 The BHW anti-unitary extension of the classical Not gate.

Taking inspiration from \([\text{14]}\) also in the anti-linear case we can consider the operator introduced by Bužek, Hillery, and Werner (BHW) in \([\text{1}]\) and defined by the law:

\[
T^a_{N_1}(|\psi\rangle) = \langle 1|\psi\rangle^*|0\rangle - \langle 0|\psi\rangle^*|1\rangle
\]

The operator \(T^a_{N_1} : \mathbb{C}^2 \rightarrow \mathbb{C}^2\) produces the transition

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow T^a_{N_1} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} := \begin{pmatrix} c_2^* \\ -c_1^* \end{pmatrix}
\]

that can be also expressed as \(T^a_{N_1}(c_1|0\rangle + c_2|1\rangle) = c_2^*|0\rangle - c_1^*|1\rangle\). \(T^a_{N_1}\) is an anti-unitary operator whose inverse (coinciding with the adjoint) is the anti-unitary operator \((T^a_{N_1})^{-1} = (T^a_{N_1})^\dagger\) defined by the transition:

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow (T^a_{N_1})^{-1} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} := \begin{pmatrix} -c_2^* \\ c_1^* \end{pmatrix}
\]

Since for any \(\psi \in \mathbb{C}^2\) one has that \(\langle \psi|T^a_{N_1}\psi\rangle = 0\), as pointed out in \([\text{1}]\) the anti-unitary operator \(T^a_{N_1}\) describes a transformation “that will take an arbitrary (unknown) qubit and transform it into the qubit orthogonal to it” (property of complementing a qubit, i.e., to transform any pure “state” \(|\psi\rangle\) into its orthogonal \(|\psi^\perp\rangle = T^a_{N_1}|\psi\rangle\)). This result cannot be achieved by any of the other possible unitary and anti-unitary extensions of the classical Not gates described before.

5 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 \(\rho\) be a density operator in the Hilbert space \(\mathbb{C}^2\). Then, we have that:

1. \(\rho \mapsto T^l_{N} \circ \rho \circ (T^l_{N})^{-1}\)

   corresponds to the transformation \((P_x, P_y, P_z) \rightarrow (P_x, -P_y, -P_z)\) in which the involved points are antipodes with respect to the \(z\) axis. In particular, any point on the \(zy\) plane of the Poincaré sphere \((0, P_y, P_z)\) is transformed into the real antipode \((0, -P_x, -P_z)\).
2. $\rho \mapsto T_{N_1}^l \circ \rho \circ (T_{N_1}^l)^{-1}$ corresponds to the transformation $(P_x, P_y, P_z) \rightarrow (-P_x, P_y, -P_z)$ 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 $T_{N_1}^l$ into its real antipodal $(-P_x, 0, -P_z)$.

3. $\rho \mapsto T_{N_1}^q \circ \rho \circ (T_{N_1}^q)^{-1}$ corresponds to transformation $(P_x, P_y, P_z) \rightarrow (P_x, P_y, -P_z)$ in which the involved points are antipodes with respect to the $xy$ plane.

4. $\rho \mapsto T_{N_1}^q \circ \rho \circ (T_{N_1}^q)^{-1}$ corresponds to the transformation $(P_x, P_y, P_z) \rightarrow (-P_x, -P_y, -P_z)$, such that all the involved pairs are antipodes of each other.

From point (4) we have that the anti–unitary BHW operator $T_{N_1}^q$ satisfy the requirement of describing the universal not gate which performs the operation of “complementing” any qubit, i.e., of transforming any qubit in a qubit orthogonal to it (operation of complementation). But, furthermore, it transforms also any mixed state in another mixed state whose Poincaré representations are antipodal between them.

From the unitary point of view, the operator more similar to $T_{N_1}^q$ is $T_{N_1}^l$ which applied to a generic vector $|\vartheta, \varphi\rangle$ (the first vector of (11)) produces the transition:

$$|\vartheta, \varphi\rangle \mapsto T_{N_1}^l |\vartheta + \pi, -\varphi\rangle = |\vartheta + \pi, -(\varphi + 2\pi)\rangle$$

(26)

In particular, one has that for any vector describing linear polarized light the following identity holds:

$$T_{N_1}^l \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix} = \begin{pmatrix} -\sin \alpha \\ \cos \alpha \end{pmatrix} = T_{N_1}^q \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix}$$

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 component 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 $\pi$ around the $y$–axis.” [3].

As pointed out before, 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. According to (U2), their inner product is

$$\langle \vartheta, \varphi | \vartheta + \pi, -\varphi \rangle = 2i \sin \varphi \cos \frac{\vartheta}{2} \sin \frac{\vartheta}{2}$$

which is trivially 0 (orthogonality) under the condition $\varphi = 0$, i.e., for any pure state whose Poincaré surface representation is on the $xz$ plane. Under this condition the above transition (26) becomes

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

Setting $\vartheta = 2\alpha$, as shown in subsection (1.1), the vector $|\alpha\rangle = |2\alpha, 0\rangle$ describes the quantum (pure) state of light linear polarized along direction $\alpha$ with respect to the reference axis $A_1$ of the analyzer Nicol prism which constitute the preparation part of the experiment. In this interpretation the linear realization $T_{N_1}^l$ 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 $\alpha$ and $\alpha + \pi/2$, for a fixed, but arbitrary $\alpha$. Let us make their generic convex combination $\rho_{\lambda,\alpha,\alpha+\pi/2} = \lambda \rho_{\alpha} + (1 - \lambda) \rho_{\alpha+\pi/2} = \frac{1}{2} [ I + (2\lambda - 1)(\sin 2\alpha \sigma_x + \cos 2\alpha \sigma_z) ]$ with $0 \leq \lambda \leq 1$. Then, the associated Poincaré representation is the point $((2\lambda - 1) \sin(2\alpha), 0, (2\lambda - 1) \cos(2\alpha))$ inside the unit $xz$ circle of $\mathbb{R}^3$, whose antipodes has as corresponding density operator just $\rho_{\lambda,\alpha+\pi/2,\alpha} = \lambda \rho_{\alpha+\pi/2} + (1 - \lambda) \rho_{\alpha} = T_{N_1}^l \circ \rho_{\lambda,\alpha,\alpha+\pi/2} \circ (T_{N_1}^l)^{-1}$.

As a conclusion, the no–go theorem about the impossibility of constructing a unitary universal NOT gate (with the BHW proposal of an anti–unitary version of gate of this kind) is a result undoubted very relevant from the mathematical point of view. It gives a profound insight about the role of universality, as condition strictly linked to the requirement of complementing a qubit. If there is some interesting physical application requiring a universal version of the classical NOT gate in the context of a single register qubit, then the answer is certainly negative. But the linear version $T_{N_1}^l$ of this NOT gate, also if it lacks of the global universality, is not so poor since all the states, either pure or mixed, of linear polarization are transformed by this quantum gate in the corresponding antipodal (and in the particular case of pure linear polarized states, in their orthogonal). So the involved physical application should be fulfilled by a linear gate, at least with respect to the very large number of states in which the condition of antipodal transformation works (all linear polarized states).

A different (similar) discourse must (can) be done in the case of coupled quantum systems described inside the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$ (2–qubits or 2–length quregister).

6 Client-server computing

Consider a wireless communication between a portable device that enables a client (say, Alice) to deliver data (e.g., prepare and send a system in a state $\eta$ and store data (e.g., measure a system and store the results). It is sometimes beneficial for a computing device to compute enough times to obtain the description of the outgoing state $\Omega(\eta)$ up to a desired degree of accuracy, where $\Omega$ is the operation described by $[7]$. It is a characteristic feature of yes-no experiments in quantum mechanics that the detection is repeated a large number of times, always preparing the system in the same way. The statements of the results are typically statistical in character: one obtain that an average of incident particles were registered by a particular yes-no detector. The single test involves only one particle, but the final report involves statistical averages of a large number of identical single experiments. In this client-server model computations take place in quantum circuits of a server (say, Bob).

Suppose Alice prepares and sends a quantum system in a state $\eta$ and by a classical communication ask Bob to compute a U-NOT gate before giving the quantum system back.

By $[1]$ the best we can obtain is $\eta_b = \frac{2}{3} \eta + \frac{i}{3} \eta$ with a fidelity of $\frac{2}{3}$. Now, suppose Bob has a NOT$^1$ gate available. In addition Alice has to communicate the polar angles $\Theta, \Phi$ and Bob has to set the polar angles $\Theta, \Phi$ of the NOT$^1$ gate (e.g., set the rotation axis). An error can occur during the communication or during the set up of the server device. Consider a generic convex combination $\eta_{\lambda,\alpha,\alpha+\pi/2} = \lambda \eta_{\alpha} + (1 - \lambda) \eta_{\alpha+\pi/2} = \frac{1}{2} [ I + (2\lambda - 1)(\sin 2\alpha \sigma_x + \cos 2\alpha \sigma_z) ]$ with $0 \leq \lambda \leq 1$. Then, the associated Poincaré representation is the point $((2\lambda - 1) \sin(2\alpha), 0, (2\lambda - 1) \cos(2\alpha))$ inside the unit $xz$ circle of $\mathbb{R}^3$, whose antipodes has as corresponding density...
operator just \( \eta_{\lambda, \alpha} = \lambda \eta_{\alpha} + (1 - \lambda) \eta_{\alpha} = T_{N_1(\Theta, \Phi)}^l \circ \eta_{\lambda, \alpha} \circ (T_{N_1(\Theta, \Phi)}^l)^{-1} \). If an error can occur during the communication or during the set up of the server device (e.g., \( x \)), else than the normalized sum of the Pauli spin matrixes along the \( x \) and \( z \) directions.

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

We will now consider two important genuine quantum gates that transform elements of the computational basis of \( \mathbb{C}^2 \) into qubits that are superpositions: the square root of the identity and the square root of the negation.

The basic property of the square root of identity gate \( T_H \) is the following:

\[
\text{for any } |\psi\rangle \in \mathbb{C}^2, \ T_H(T_H(|\psi\rangle)) = |\psi\rangle.
\]

The basic property of the square root of Not gate \( T_{\sqrt{N}} \) is the following:

\[
\text{for any } |\psi\rangle \in \mathbb{C}^2, \ T_{\sqrt{N}}(T_{\sqrt{N}}(|\psi\rangle)) = T_N(|\psi\rangle).
\]

In other words, applying twice the square root of the negation means negating.

Any quantum, either unitary or anti-unitary, realization of the square root of identity (also Walsh-Hadamard) gate \( T_H \) and of the square root of Not gate \( T_{\sqrt{N}} \) on the Hilbert space \( \mathbb{C}^2 \) must satisfy the minimal conditions [13] translated to the present cases and extended to the whole Hilbert space \( \mathbb{C}^2 \) following [12].

In this way, this transformation turns out to be unitary or anti-unitary according to the linear or anti-linear extension of \( T_H \) and \( T_{\sqrt{N}} \) to any vector \( |\psi\rangle \in \mathbb{C}^2 \) such that \( |\psi\rangle = \langle 0|\psi\rangle |0\rangle + \langle 1|\psi\rangle |1\rangle \).

7.1 Linear extensions of the square root of identity gate.

In this subsection we introduce a linear extension of the above minimal rules describing the square root of identity gate.

\[
T_H^l(|\psi\rangle) = \langle 0|\psi\rangle \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) + \langle 1|\psi\rangle \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}}[(\langle 0|\psi\rangle + \langle 1|\psi\rangle) |0\rangle + (\langle 0|\psi\rangle - \langle 1|\psi\rangle) |1\rangle]
\]

(27)

For \( c_1 = \langle 0|\psi\rangle \) and \( c_2 = \langle 1|\psi\rangle \), the operator \( T_H^l : \mathbb{C}^2 \rightarrow \mathbb{C}^2 \) produces the transformation

\[
\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \rightarrow T_H^l \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} c_1 + c_2 \\ c_1 - c_2 \end{pmatrix}
\]

(28)

that can be also expressed as \( T_H^l(c_1 |0\rangle + c_2 |1\rangle) = \frac{1}{\sqrt{2}}[(c_1 + c_2) |0\rangle + (c_1 - c_2) |1\rangle] \). The operator \( T_H^l \) is unitary with (unitary) inverse \( (T_H^l)^{-1} = (T_H^l)^\dagger = T_H^l \) and is defined by the matrix

\[
T_H^l = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)
\]

(29)

This unitary operator describes in this way a self–reversible quantum gate, which is nothing else than the normalized sum of the Pauli spin matrixes along the \( x \) and \( z \) directions.
7.2 The anti–linear extension of the square root of identity gate.

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

\[ T_H^a(|\psi\rangle) := \frac{1}{\sqrt{2}}[(|0\rangle + \langle 1\rangle^*\langle 0\rangle + (\langle 0\rangle^* - \langle 1\rangle)|1]\] (30)

The operator \( T_H^a : \mathbb{C}^2 \mapsto \mathbb{C}^2 \) produces the transition

\[
\begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} \longrightarrow T_H^a \begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  c_1 + c_2^* \\
  -c_2 + c_1^*
\end{pmatrix}
\] (31)

that can be also expressed as \( T_H^a(c_1 |0\rangle + c_2 |1\rangle) = \frac{1}{\sqrt{2}}[(c_1 + c_2^*) |0\rangle + (-c_2 + c_1^*) |1\rangle] \). \( T_H^a \) is a self–reversible anti-unitary operator: \( (T_H^a)^{-1} = (T_H^a)^\dagger = T_H^a \).

The anti–unitary operator \( T_H^a \) describes a transformation “that will take an arbitrary (unknown) qubit \( \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \) and transform it into an equally superposition of the qubit \( \sigma_z \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} c_1 \\ -c_2 \end{pmatrix} \) and the qubit orthogonal to it”.

7.3 Linear and anti–linear extensions of the square root of Not gate.

Finally, we introduce a linear extension of the above minimal rules describing the square root of Not gate.

\[
T_{\sqrt{N}}^l(|\psi\rangle) = \langle 0\rangle \left( \frac{1+i}{\sqrt{2}} |0\rangle + \frac{1-i}{\sqrt{2}} |1\rangle \right) + \langle 1\rangle \left( \frac{1+i}{\sqrt{2}} |0\rangle + \frac{1-i}{\sqrt{2}} |1\rangle \right)
\]

\[
= \frac{1}{2} \left( (1+i)\langle 0\rangle |\psi\rangle + (1-i)\langle 1\rangle |\psi\rangle \right) \langle 0\rangle + \langle 1\rangle \left( (1+i)(0\rangle |\psi\rangle + (1+\text{i})|1\rangle |\psi\rangle \right) |1\rangle.
\]

The operator \( T_{\sqrt{N}}^l : \mathbb{C}^2 \mapsto \mathbb{C}^2 \) corresponds to transformation

\[
\begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} \longrightarrow T_{\sqrt{N}}^l \begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
  (1+i)c_1 + (1-i)c_2 \\
  (1-i)c_1 + (1+i)c_2
\end{pmatrix}
\] (32)

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

\[
T_{\sqrt{N}}^a(|\psi\rangle) = \frac{1}{\sqrt{2}}[(|0\rangle - \langle 1\rangle^*|0\rangle + (\langle 0\rangle^* + \langle 1\rangle)|1]\] (33)

The operator \( T_{\sqrt{N}}^a : \mathbb{C}^2 \mapsto \mathbb{C}^2 \) corresponds to the transformation

\[
\begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} \longrightarrow T_{\sqrt{N}}^a \begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  c_1 - c_2^* \\
  c_2 + c_1^*
\end{pmatrix}
\] (34)

The anti–unitary operator \( T_{\sqrt{N}}^a \) describes a transformation “that will take an arbitrary (unknown) qubit and transform it into an equally superposition of the qubit and the qubit orthogonal to it”.

8 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 $|\psi\rangle \rightarrow |\psi^\perp\rangle$ 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 $T^{l}_{N_1}$ realizes the quantum computational Not gate perfectly, but it is not a universal one.

On the other side, the BHW operator $T^{a}_{N_1}$ 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 loose the possibility to realize a quantum not gate: there is no physical operation which can implement such transformation. In particular, given a quantum computational network, we can think about a logical gate as a device which performs a given operation on selected qubits in a fixed period of time: so a quantum Not gate must be a completely positive trace preserving operator and any anti–unitary operation, as $T^{a}_{N_1}$, is not completely positive.

We suggest that the above analysis introduces a new point of view on complementarity in quantum computational theory that is added to the notion of complementarity between quantum and classical information introduced by Oppenheim et al. in [17] and M. Horodecki et al. in [18]. Let us briefly remember that the Bohr’s complementarity applies to properties of the system that are observable and the logical relations that this concept represents are about the mutual exclusion of physical system’s descriptions. Differently from the Bohr’s idea, the notion of complementarity we want to introduce is not related to outcomes of measurements, but it regards two complementary ways to describe the process to complement the information encoded in a two level quantum system: unitary and anti-unitary one. From the point of view of the unitary description of complementing a qubit, there is the unitary operator $T^{l}_{N_1}$ that is physically feasible: it implements a quantum not gate that acts on a considerable set of states (for instance at least all possible, either pure or mixed, states of linearly polarizations light), but at the same time it is not universal since we loose the possibility to complement any qubit with the best fidelity. From the point of view of the anti-unitary description, there is the operator $T^{a}_{N_1}$ that perfectly maps every point on the Poincaré sphere onto its diagonally opposite point with the best fidelity, but we loose the possibility of any physical implementation of the gate. In this last case a possible solution comes from the quantum not gate introduced by Buzek-Hillery-Werner that approximates the anti-unitary transformation $T^{a}_{N_1}$ 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 $\frac{2}{3}$ [1].

1. V. Bužek and M. Hillery and R. F. Werner (1999), Optimal manipulations with qubits: Universal-NOT gate, Phys. Rev. A, 60, pp. 2626-2629.
2. N. Gisen and S. Popescu (1999), Spin flips and quantum information for antiparallel spins, Phys. Rev. Lett., 83, pp. 432-435.
3. V. Bužek and M. Hillery and R. F. Werner (2000), Universal-NOT gate, Journal of Modern Optics, 47, pp. 211-232.
4. N. Gisen (2002), *NOT logic*, Nature, 419, pp. 797-728.
5. F. De Martini and V. Bužek and F. Sciarrino and C. Sias (2002), *Experimental realization of the quantum universal Not gate*, Nature, 419, pp. 815-818.
6. M. A. Nielsen and I. L. Chuang (2000), *Quantum Computation and Quantum Information*, Cambridge Univ. Press (Cambridge).
7. D. Bouwmeester, A. Ekert and A. Zeilinger (2000), *The Physics of Quantum Information*, Springer-Verlag (Berlin).
8. U. Fano (1957), *Description of States in Quantum Mechanics by Density Matrix and Operator Techniques*, Reviews of Modern Physics, 29, pp. 74-93.
9. U. Fano (1949), *Remarks on the Classical and Quantum Mechanical Treatment of Partial Polarisation*, Journal of the Optical Society of America, 39, pp. 859-863.
10. E. P. Wigner (1931), *Gruppentheorie*, Frederick Vieweg und Sohn (Braunschweig), English translation: *Group Theory*, Academic Press Inc., NY, 1959.
11. V. Bargmann (1964), *Note on Wigner’s theorem on symmetry operations*, J. Math. Phys., 5, pp. 862-868.
12. B. Mielnik (1969), *Theory of Filters*, Commun. Math. Phys., 15, pp. 1-46.
13. E. B. Davies (1976), *Quantum Theory of Open Systems*, Academic Press (New York).
14. R. Landauer (1961), *Irreversibility and heat generation in the computing process*, IBM J. Res. Dev., 36, pp. 183-191.
15. C. H. Bennett (1973), *Logical reversibility of computation*, IBM J. Res. Dev., 17, pp. 525-532.
16. C. H. Bennett (1988), *Notes on the history of reversible computation*, IBM J. Res. Dev., 32, pp. 16-23.
17. H. S. Leff and A. F. Rex (1990), *Maxwells Demon: Entropy, Information, Computing*, Princeton University Press (Princeton).
18. J. Oppenheim, K. Horodecki, M. Horodecki, P. Horodecki, R. Horodecki (2003), *Mutually exclusive aspects of information carried by physical systems: Complementarity between local and nonlocal information*, Phys. Rev. A, 68, pp. 022307 1-13.
19. M. Horodecki, P. Horodecki, R. Horodecki (2004), *Quantum information isomorphism, beyonf the dilemma of the Scylla ontology and the Charybdis of instrumentalism*, IBM Journal of Research and development, 48, issue 1 pp. 139-147.