GEOMETRICAL REPRESENTATION OF QUANTUM BIT OPERATIONS

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Reprezentările grafice bazate pe transformări geometrice sunt o metodă expresivă foarte bună de simulare a operațiilor efectuate asupra sistemelor cuantice de procesare a informației. Considerând un sistem format dintr-un sigur qubit, demonstrațiile prezentate în această lucrare justifică corespondența între o clasă de operații care modifică starea qubitului şi nişte tranformări geometrice pe sfera Bloch.

Operațiile efectuate asupra qubitului sunt expimate prin exponențierea operatorilor Pauli, în timp ce transformările geometrice corespunzătoare sunt rotații pe sfera Bloch, în jurul axelor de coordonate.

Graphical representations based on geometrical transformations are a very expressive method of simulating the operations performed on quantum information processing systems. Considering a single qubit system, the proofs given in this paper justify the correspondence between a class of operations that modify the qubit state and some geometrical transformations on the Bloch sphere.

The single qubit operations are expressed by the exponentiation of Pauli operators, whereas the corresponding geometrical transformations are rotations on the Bloch sphere around the coordinate axes.

Keywords: quantum computing, rotation operators, Bloch sphere

1. Introduction

Quantum computing studies information processing tasks that can be implemented based on physical systems obeying the quantum mechanical laws, as they are currently formulated in the mainstream physics science. This is a relatively new field of study, which was launched following some great breakthroughs in the area of theoretical computer science. These allowed theoreticians to raise challenges against the strong version of the Church – Turing thesis and to propose a different thesis, based on the quantum computing paradigme.

This new thesis [1] is now known as the strong Church – Turing – Deutsch thesis and it postulates that any algorithmic physical process can be efficiently simulated (or implemented) on a quantum computer.

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A few algorithms to sustain this thesis have been already demonstrated [2] but the quantum computing field itself still has to deal with important issues related to physical implementation of the so called quantum computing machines. The biggest challenge is represented by the difficult manipulation of quantum systems that must ensure errors are kept at reasonable levels [3].

Until these implementation challenges are overcome, the obvious approach used for advancing the quantum algorithms research is to use simulations that use classical machines (ordinary computers) to emulate quantum processing tasks. This is where the graphical representation of the operations taken place during the simulation may prove useful.

Starting from the simplest quantum processing system, based on a single qubit, the proofs in following chapters justify the correspondence between a class of operations that transform the qubit state and the geometry on a sphere, the Bloch sphere.

The qubit operations are expressed by the exponentiation of Pauli operators [4], which form an orthogonal basis for the vector space defined by the set of linear operators acting on a single qubit. The corresponding geometrical transformations are simple rotations on the Bloch sphere around the coordinate axes.

2. Qubits in a pure state – Bloch sphere

Using the well established Dirac notation [5], the pure state of a qubit, defined as a linear superposition of the computational basis states, it is represented by the following equation:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \qquad \alpha, \beta \in \mathbf{C}, \qquad |\alpha|^2 + |\beta|^2 = 1, \tag{1}$$

where $|0\rangle$ and $|1\rangle$ are the computational basis states. So, a qubit in a pure state is represented by a unit vector in a bi-dimensional complex vector space.

For the purpose of geometrical representation, it is more useful to use the polar coordinates for complex numbers. Considering also the measuring principle from quantum mechanics stating that measuring two quantum states that differ only by a global phase factor, provides always the same result ($|\psi\rangle \cong \mathrm{e}^{i\phi}|\psi\rangle$, $\forall \phi \in \mathbf{R}$), the state of the qubit can be then expressed as:

$$|\psi\rangle = \cos\frac{\gamma}{2}|0\rangle + \sin\frac{\gamma}{2}\mathrm{e}^{i\varphi}|1\rangle \qquad \gamma \in [0, \pi], \;\; \varphi \in [0, 2\pi) \tag{2}$$

This equation represents therefore the base starting point that provides for a geometrical representation of qubit states, because it proves that there is a bijective mapping between the set of measurable pure states of a qubit and the unit sphere in the Euclidean tridimensional space. According to this mapping, each and every pure qubit state defined by equation (1) has an associated point P on the unit sphere, a point having the spherical coordinates $P(\varphi,\gamma)$. The $\overline{OP}$ vector, with the origin in the center of the unit sphere, is called "*Bloch vector*" and has the following coordinates in a tri-dimensional Euclidean space [4]:

$$(p_x, p_y, p_z) = (\cos\varphi\sin\gamma, \sin\varphi\sin\gamma, \cos\gamma) \quad (3)$$

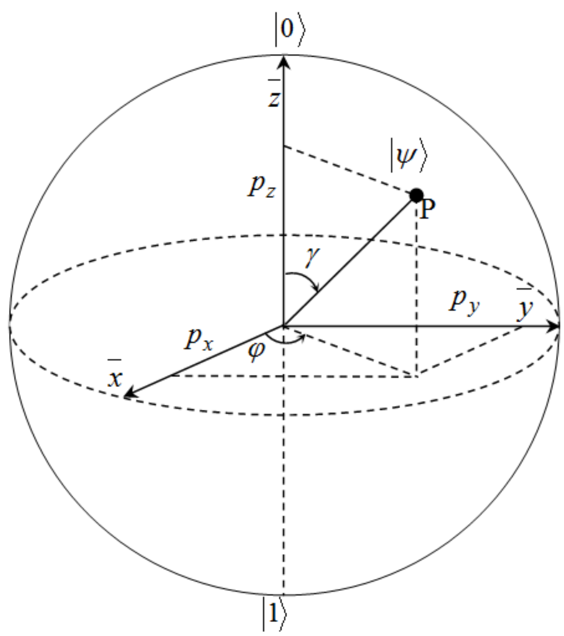

Fig. 1. A qubit pure state represented on the Bloch sphere

3. Qubits in a mixed state – Bloch ball

As opposed to pure state qubits, where a state vector is used to represent their state, when the qubit state is mixed, the density operator is used for representing that state. Actually, these two representations are mathematically equivalent, but they have different, though similar, physical interpretations. The principles that form the base for the quantum mechanics theory can be formulated using either of the two approaches: state vectors or density operators.

Assuming a quantum system is in an unknown state, but the possible states form a finite and discrete set, where the pure state $|\psi_i\rangle$ occurs with the probability p_i, the density operator associated with that system is defined by the following equation:

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad 0 \le p_i \le 1, \quad \sum_i p_i = 1 \tag{4}$$

The density operator is a self-adjoint (Hermit) positive operator, with unit norm:

$$\begin{aligned}
&\rho^\dagger \equiv \sum_i p_i^* |\psi_i\rangle\langle\psi_i| = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \rho \\
&\langle\psi|\rho|\psi\rangle = \sum_i p_i \langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle = \sum_i p_i \langle\psi|\psi_i\rangle\langle\psi|\psi_i\rangle^* = \sum_i p_i \left|\langle\psi|\psi_i\rangle\right|^2 \ge 0 \\
&\mathrm{tr}(\rho) = \mathrm{tr}\left(\sum_i p_i |\psi_i\rangle\langle\psi_i|\right) = \sum_i p_i \,\mathrm{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i = 1
\end{aligned} \tag{5}$$

According to the quantum mechanics formalism based on density operators, the pure states are just a particular case that can be also represented by density operators. The density operator of a pure state is defined as:

$$\rho \equiv |\psi\rangle\langle\psi| \tag{6}$$

The trace of a general density operator satisfies the following inequality; with the equality happening if and only if the respective density operator represents a pure state:

$$\mathrm{tr}(\rho^2) \le 1 \tag{7}$$

For the quantum system representing one qubit, the associated density operator ρ belongs to the complex vector space defined by the set of all operators generated by the Pauli operators. Therefore that density operator can be decomposed as a linear superposition of the Pauli operators, using complex coefficients:

$$\rho = aI_2 + b\sigma_x + c\sigma_y + d\sigma_z, \qquad a,b,c,d \in \mathbf{C} \tag{8}$$

The complex coefficients can be further refined by imposing the restrictions that apply to density operators: self-adjoint, positive and unitary. Hence the equation above can be transformed such that it allows for a geometrical representation:

$$\rho = \frac{1}{2}\left(I_2 + r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right) = \frac{1}{2}\left(I_2 + \bar{r}\cdot\bar{\sigma}\right) \tag{9}$$

whereas $\bar{r}$ is a vector in the real tri-dimensional Euclidian space. Considering the matrix associated with this density operator in the computational basis state, and by forcing its eigenvalues to be real positive numbers (this is allowed because the operator is itself positive), it follows that the $\bar{r}$ vector is restricted to a unitary ball, centered in the origin:

$$r_x^2 + r_y^2 + r_z^2 \le 1 \Leftrightarrow \left\|\bar{r}\right\| \le 1 \tag{10}$$

Again, the equality happens if and only if the respective density operator represents a pure state. The north and south poles of the ball represent two particular pure states: the computational basis states.

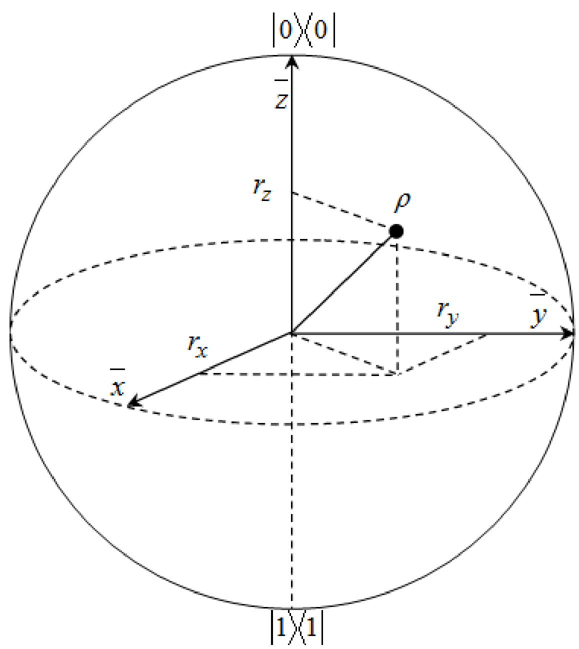

Fig. 2. A density operator represented on the Bloch ball

4. Rotation operators

The Pauli operators can be used to define a special set of operators, which have a very special meaning for the quantum computation: the rotation operators. These definitions rely on the properties of matrix exponentiation, which is defined using the Taylor-Maclaurin series.

The complex exponential function can be defined on the space of square matrices with dimension n x n using a Taylor-Maclaurin formula analogous to scalar complex functions:

$$\exp(iAx) = \sum_{k=0}^{\infty} \frac{(iAx)^k}{k!}, \qquad A \in \mathbf{M}_{n,n}, \qquad x \in \mathbf{R} \tag{11}$$

If furthermore, A is a special matrix whose square power is the identity matrix:

$$A^2 = I_n \Rightarrow A^{2k} = I_n; A^{2k+1} = A, \forall k \in N \tag{12}$$

then the Taylor-Maclaurin (11) can be further refined as follows:

$$\begin{aligned} \exp(iAx) &= I_n + \frac{1}{1!} iAx + \frac{1}{2!} i^2 A^2 x^2 + \frac{1}{3!} i^3 A^3 x^3 + \frac{1}{4!} i^4 A^4 x^4 + \frac{1}{5!} i^5 A^5 x^5 + \ldots.. \\ &= \sum_{k=0}^{\infty} \left(\frac{1}{(2k)!} i^{2k} x^{2k} I_n + \frac{1}{(2k+1)!} i^{2k+1} x^{2k+1} A \right) = \\ &= \sum_{k=0}^{\infty} \left((-1)^k \frac{1}{(2k)!} x^{2k} I_n + i(-1)^k \frac{1}{(2k+1)!} x^{2k+1} A \right) \end{aligned} \tag{13}$$

Using the Taylor-Maclaurin formulas for trigonometric functions:

$$\begin{aligned} \cos(x) &= \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k)!} x^{2k} = 1 - \frac{1}{2!} x^2 + \frac{1}{4!} x^4 - \frac{1}{6!} x^6 + \ldots.. \\ \sin(x) &= \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k+1)!} x^{2k+1} = x - \frac{1}{3!} x^3 + \frac{1}{5!} x^5 - \frac{1}{7!} x^7 + \ldots.. \end{aligned} \tag{14}$$

it can be deducted that the two series in equation (13) are convergent and their sums are the trigonometric functions as defined by (14):

$$\exp(iAx) = \left(\sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k)!}x^{2k}\right)I_n + i\left(\sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k+1)!}x^{2k+1}\right)A = \\ = \cos(x)I_n + i\sin(x)A \tag{15}$$

Now, because the Pauli matrices satisfy the equation (12), it means they can be substituted in equation (15), the resulting exponentials being the very rotation matrices, whose corresponding operators can be thus defined as:

$$R_k(\theta) \equiv \exp\left(\frac{-i\theta\sigma_k}{2}\right) = \cos\frac{\theta}{2}I_2 - i\sin\frac{\theta}{2}\sigma_k, \forall k = \overline{0,3} \tag{16}$$

4.1. Rotation operator on *z* axis

For the $k = 3$ case in equation (16), the operator and its associated matrix, according to the computational basis state, defined by the following equation:

$$R_z(\theta) \equiv \exp\left(\frac{-i\theta Z}{2}\right) = \cos\frac{\theta}{2}I_2 - i\sin\frac{\theta}{2}Z = \begin{bmatrix} \mathrm{e}^{\frac{-i\theta}{2}} & 0 \\ 0 & \mathrm{e}^{\frac{i\theta}{2}} \end{bmatrix} \tag{17}$$

has the following geometrical interpretation: for a qubit in a pure state, described by the equation (2), upon which an operation defined by equation (17) is performed such that the qubit transformed state is:

$$|\psi_1\rangle = R_z(\theta)|\psi_0\rangle = \cos\frac{\gamma_1}{2}|0\rangle + \sin\frac{\gamma_1}{2}\mathrm{e}^{i\varphi_1}|1\rangle \tag{18}$$

and if the corresponding points on the Bloch sphere, P_0 and P_1, for the initial state and respectively for the transformed state are defined by equation (3), then P_1 can be deducted geometrically by rotating P_0 with angle θ around the *z* axis.

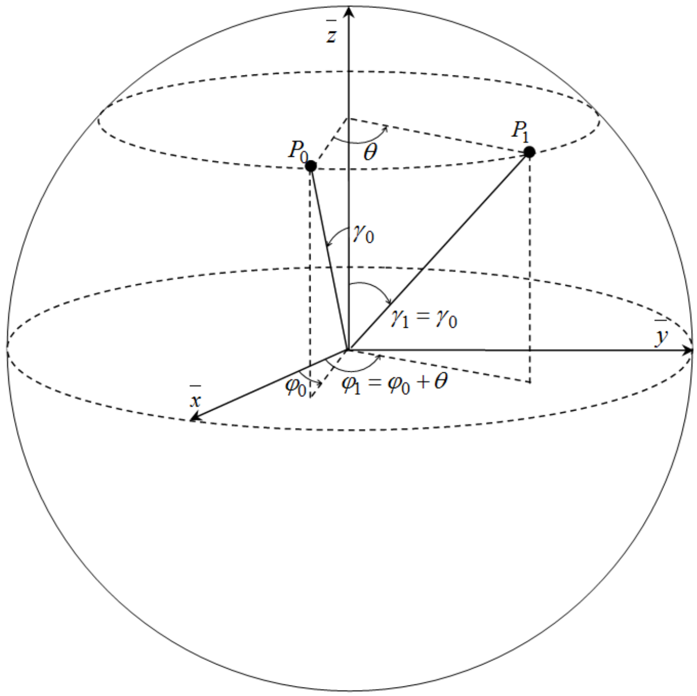

Fig. 3. Geometrical representation of the R_z operator

This interpretation can be validated by simply applying the operator on the qubit in initial state:

$$R_z(\theta)|\psi_0\rangle = \begin{bmatrix} e^{\frac{-i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{bmatrix} \begin{bmatrix} \cos\frac{\gamma_0}{2} \\ \sin\frac{\gamma_0}{2} e^{i\varphi_0} \end{bmatrix} = \begin{bmatrix} \cos\frac{\gamma_0}{2} e^{\frac{-i\theta}{2}} \\ \sin\frac{\gamma_0}{2} e^{i\varphi_0} e^{\frac{i\theta}{2}} \end{bmatrix} = \tag{19}$$

$$= e^{\frac{-i\theta}{2}} \begin{bmatrix} \cos\frac{\gamma_0}{2} \\ \sin\frac{\gamma_0}{2} e^{i(\varphi_0+\theta)} \end{bmatrix} = e^{\frac{-i\theta}{2}} \begin{bmatrix} \cos\frac{\gamma_1}{2} \\ \sin\frac{\gamma_1}{2} e^{i\varphi_1} \end{bmatrix} = e^{\frac{-i\theta}{2}} |\psi_1\rangle \cong |\psi_1\rangle$$

and observing on the Fig. 3. the parameters for the transformed state:

$$P_0 \to P_1 \Leftrightarrow \gamma_1 = \gamma_0 \text{ şi } \varphi_1 = \varphi_0 + \theta \tag{20}$$

4.2. Rotation operator on *x* axis

For the $k = 1$ case in equation (16), the operator and its associated matrix, according to the computational basis state, defined by the following equation:

$$R_x(\theta) \equiv \exp\left(\frac{-i\theta X}{2}\right) = \cos\frac{\theta}{2} I_2 - i\sin\frac{\theta}{2} X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{21}$$

has the following geometrical interpretation: for a qubit in a pure state, described by the equation (2), upon which an operation defined by equation (17) is performed such that the qubit transformed state is:

$$|\psi_1\rangle = R_x(\theta)|\psi_0\rangle = \cos\frac{\gamma_1}{2}|0\rangle + \sin\frac{\gamma_1}{2} e^{i\varphi_1}|1\rangle \tag{22}$$

and if the corresponding points on the Bloch sphere, P_0 and P_1, for the initial state and respectively for the transformed state are defined by equation (3), then P_1 can be deducted geometrically by rotating P_0 with angle θ around the x axis.

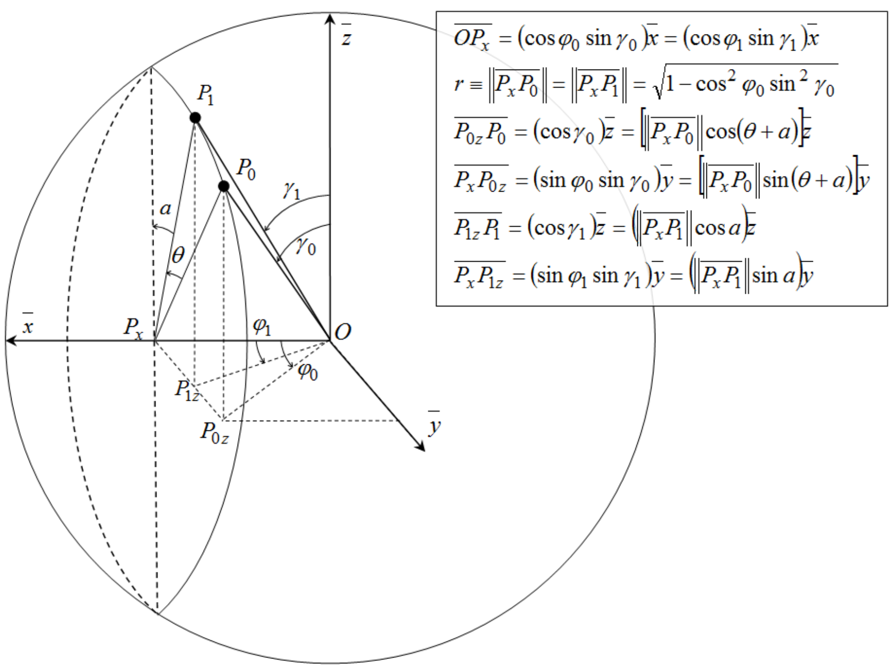

Fig. 4. Geometrical representation of the R_x operator

4.3. Rotation operator on *y* axis

For the $k = 2$ case in equation (16), the operator and its associated matrix, according to the computational basis state, defined by the following equation:

$$R_y(\theta) \equiv \exp\left(\frac{-i\theta Y}{2}\right) = \cos\frac{\theta}{2} I_2 - i \sin\frac{\theta}{2} Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{23}$$

has the following geometrical interpretation: for a qubit in a pure state, described by the equation (2), upon which an operation defined by equation (17) is performed such that the qubit transformed state is:

$$|\psi_1\rangle = R_y(\theta)|\psi_0\rangle = \cos\frac{\gamma_1}{2}|0\rangle + \sin\frac{\gamma_1}{2} e^{i\varphi_1}|1\rangle \tag{24}$$

and if the corresponding points on the Bloch sphere, P_0 and P_1, for the initial state and respectively for the transformed state are defined by equation (3), then P_1 can be deducted geometrically by rotating P_0 with angle θ around the *y* axis.

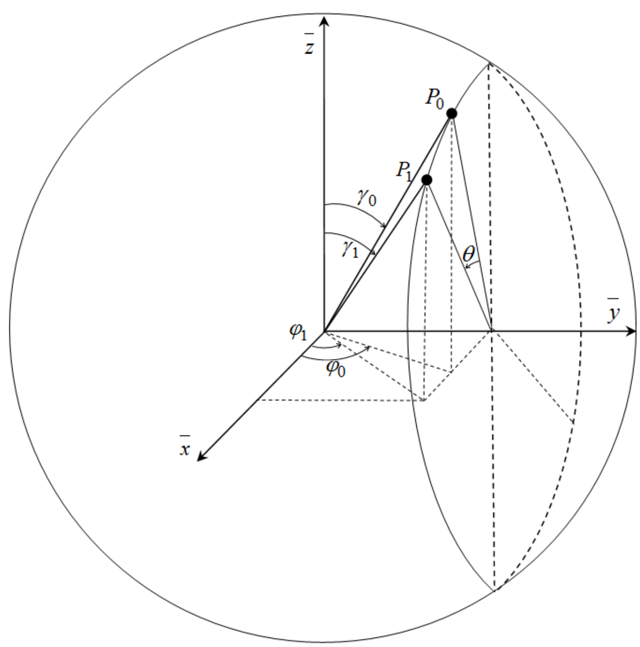

Fig. 5. Geometrical representation of the R_y operator

For validating this last geometrical representation, one can make use of the two representations demonstrated in the previous two chapters, for R_x and R_z. Any rotation with angle θ around the y axis can be factored out into three rotations made in the following order:

- one rotation with angle $-\frac{\pi}{2}$ around the $\bar{z}$ axis
- one rotation with angle θ around the $\bar{x}$ axis
- one rotation with angle $\frac{\pi}{2}$ around the $\bar{z}$ axis

Then, according to the previous two geometrical representations, these three rotations can be written using the respective operators:

$$R_z\left(\frac{\pi}{2}\right)R_x(\theta)R_z\left(-\frac{\pi}{2}\right)=\begin{bmatrix} e^{-i\frac{\pi}{4}} & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}\begin{bmatrix} e^{i\frac{\pi}{4}} & 0 \\ 0 & e^{-i\frac{\pi}{4}} \end{bmatrix}=$$

$$=\begin{bmatrix} e^{-i\frac{\pi}{4}} & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}\begin{bmatrix} e^{i\frac{\pi}{4}}\cos\frac{\theta}{2} & -e^{i\frac{\pi}{4}}\sin\frac{\theta}{2} \\ e^{-i\frac{\pi}{4}}\sin\frac{\theta}{2} & e^{-i\frac{\pi}{4}}\cos\frac{\theta}{2} \end{bmatrix}=\begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}=R_y(\theta)$$

6. Conclusions

Starting from the simplest quantum processing system, based on a single qubit, the proofs together with the diagrams presented above, justify the correspondence between an important class of operations that transform the qubit state and the geometry on a sphere, the Bloch sphere.

The qubit operations are expressed by the exponentiation of Pauli operators, which form an orthogonal basis for the vector space defined by the set of linear operators acting on a single qubit. Because the Pauli operators form such a basis set, it follows that they can be used to factor any unitary operator. And therefore, any single qubit operator can be given a geometrical representation.

The corresponding geometrical transformations are simple rotations on the Bloch sphere around the coordinate axes. And because these rotations can be composed into any arbitrary rotation on the Bloch sphere, it follows that the geometrical representation can be generalized to any type of one qubit operator and any kind of rotation on the Bloch sphere (i.e. the rotation axis doesn't need to be a coordinate axis).

There is one limitation to this geometrical representation model though: it can be used only for operators on one qubit. There is no known generalization for quantum information processing systems composed of an arbitrary number of qubits.

But as long as the processing tasks that take place can be split in independent operators that transform only just one single qubit, a graphical representation can be given that consists of several Bloch spheres that are rotated in parallel. And there are indications that this assumption is not very farfetched, because according to the quantum circuit model, the single qubit gates together with the CNOT gates form a universal set for quantum computation [6]. That is, any quantum computation could be simulated using only single qubit operators and CNOT operators. And therefore a vast majority of the operations that take place in a multiple qubits computational task can be given a geometrical representation on multiple Bloch spheres.

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