Quantum mechanical modeling of the CNOT (XOR) gate

Miroljub Dugić

Faculty of Science, Dept. Phys., P.O.Box 60, 34 000 Kragujevac, Yugoslavia
E-mail: dugic@uis0.uis.kg.ac.yu

Abstract: We consider the CNOT quantum gate as a physical action, i.e. as unitary in time evolution of the two-qubit system. This points to the modeling of the interaction Hamiltonian of the two-qubit system which would correspond to the CNOT transformation; the analysis naturally generalizes to the Toffoli gate. Despite nonuniqueness of the model of the interaction Hamiltonian, the analysis distinguishes that the interaction Hamiltonian does not posses any global (rotational) symmetry. This forces us to conclude that the direct (non-mediated) interaction in the two-qubit system does not suffice for implementing the CNOT gate. I.e., so as to be able successfully to implement the CNOT transformation, a mediator (i.e. an external physical system interacting with both of the qubits) is required.

1. Introduction

Here we pose the question of quantum mechanical modeling of the CNOT (XOR) gate. The physical background is rather obvious: if one should like to physically implement the CNOT transformation of the two-qubit states, the CNOT action must be considered as a physical dynamics of the two-qubit (2Q) system. That is, quantum mechanically, the CNOT action represents a dynamical change of the states of the 2Q system.

For the isolated 2Q system, the evolution in time (dynamics of the system) is governed by the Schrodinger law, i.e. with the unitary in time evolution operator, \( \hat{U}(t) \). Therefore, the quantum modeling of the CNOT gate is a task of modeling the Hamiltonian of the 2Q system, so as to one may write:

\[
\hat{U}_{\text{CNOT}} = \hat{U}(t),
\]

where \( \hat{U}_{\text{CNOT}} \) is the unitary-operator representation of the logically defined the CNOT transformation.

Physically, the task (1) refers to the practical, experimental realisation of the mathematically defined the CNOT transformation.

2. Quantum mechanical form of the CNOT transformation

Usually, the CNOT (XOR) gate (transformation) is defined [1] by the unitary matrix:

\[
U_{\text{CNOT}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix},
\]

(2)
but bearing in mind that this representation refers to the "standard (computational basis"
{\mid i\rangle_1 z \otimes \mid j\rangle_2 z, i, j = 0, 1} of the 2Q system consisting of the mutually identical qubits; the
states \mid i\rangle_{\alpha z}, \alpha = 1, 2 are the eigenstates of the \(z\)-projection(s) of the spin(s), \(\hat{S}_{\alpha z}\):

\[
\hat{S}_{\alpha z} \mid 0\rangle_{\alpha z} = \frac{\hbar}{2} \mid 0\rangle_{\alpha z}
\]

(3)

\[
\hat{S}_{\alpha z} \mid 1\rangle_{\alpha z} = -\frac{\hbar}{2} \mid 1\rangle_{\alpha z}
\]

However, this representation is not very informative.

We shall start from the logical (physical) definition of the CNOT transformation, obtaining its the operator form, \(\hat{U}_{\text{CNOT}}\). This will be the basis for solving the task eq. (1).

Physically (logically), the CNOT gate is defined [1] as follows:

Acting on the states from the "computational basis" (cf. above), it does not change the state of the first ("controlled") qubit, but reverses the state of the second ("target") qubit iff the state of the first qubit is \(\mid 1\rangle_2 z\).

Formally, it reads:

\[
\hat{U}_{\text{CNOT}} \mid 0\rangle_1 z \mid j\rangle_2 z = \mid 0\rangle_1 z \mid j\rangle_2 z, \quad j = 0, 1
\]

(4)

\[
\hat{U}_{\text{CNOT}} \mid 1\rangle_1 z \mid j\rangle_2 z = \mid 1\rangle_1 z \mid \neg j\rangle_2 z, \quad j = 0, 1
\]

where "\(\neg j\)" means "not \(j\)": "not 0" = 1, and "not 1" = 0; we omit the sign of the "direct product", \(\otimes\).

With some care, but without particular difficulties, one obtains unique operator form of \(U_{\text{CNOT}}\):

\[
\hat{U}_{\text{CNOT}} = \hat{P}_1 z \otimes \hat{I}_2 + \hat{P}_2 z \otimes \hat{\sigma}_2 x,
\]

(5)

where we used the well known equality:

\[
\hat{\sigma}_x \mid j\rangle_z = \mid \neg j\rangle_z.
\]

(6)

and \(\hat{P}_1 z = \mid 0\rangle_1 z 1_z \langle 0\mid, \hat{P}_2 z = \mid 1\rangle_1 z 1_z \langle 1\mid\).

The expression (5) is the main result of this section.

3. The task

Now, the task (1) reduces to obtaining equality:

\[
\hat{U}(t) = \hat{P}_1 z \otimes \hat{I}_2 + \hat{P}_2 z \otimes \hat{\sigma}_2 x,
\]

(7)

where \(\hat{U}(t)\) represents the unitary in time evolution operator of the 2Q system.
I.e., the task is to construct a model of the Hamiltonian of the 2Q system, which satisfies:

\[
\frac{i\hbar}{\partial t} \hat{U}(t) = \hat{H}(t)\hat{U}(t),
\]

(8)

so as to fulfill eq. (7).

For simplicity, and in accordance with the quantum measurement and the decoherence theory [2-4], we shall consider the interaction Hamiltonian as the dominant term in the Hamiltonian of the system. Then we consider

\[
\hat{U}(t) \sim \hat{U}_{int}(t),
\]

(9)

where \(\hat{U}_{int}(t)\) is "generated" by \(\hat{H}_{int}\). [Notice that this simplification becomes exact in the "interaction picture", where:

\[
\frac{i\hbar}{\partial t} \hat{U}_{int} = \hat{H}_{int}\hat{U}_{int},
\]

(10a)

and

\[
\hat{H}_{int} \equiv \hat{U}_{\circ}^\dagger \hat{H}_{int}\hat{U}_{\circ}.
\]

(10b)

]

So, our task is to find a model of \(\hat{H}_{int}\), which would satisfy:

\[
\frac{i\hbar}{\partial t} \hat{U}_{int} = \hat{H}_{int}\hat{U}_{int},
\]

(11)

but so that one may write (cf. eq. (7)):

\[
\hat{U}_{int}(t) = \hat{P}_1 \otimes \hat{I}_2 + \hat{P}_2 \otimes \hat{\sigma}_2.
\]

(12)

4. Doing the task

Certainly, from eq. (11) it follows:

\[
\hat{U}_{int}(t) = \exp\{\frac{-i}{\hbar} \int_0^t \hat{H}_{int}(t') dt'/\hbar\}.
\]

(13)

Now one meets the next problem: the l.h.s. of eq. (12) exhibits the time dependecne, while the r.h.s. does not.

This problem can be resolved in few ways. Instead of being exhaustive, here we shall consider the simplest model of the time independent interaction, so as one may easily overcome the time dependence of the l.h.s. of eq. (13).

We admit that duration of the interaction is \(\tau\), i.e., that

\[
\hat{H}_{int} = \hat{V} \quad \text{for} \quad t \in [0, \tau], \text{otherwise} \hat{H}_{int} = 0.
\]

(14)
Certainly, then (13) reads:

\[ \hat{U}(t) = \exp\{-i\tau \hat{V} / \hbar\}, \quad \tau - fixed \]  

(15)

assuming that the effect of \( \hat{U}(t) \) on the initial state of the 2Q system, is not completed before \( t \approx \tau \). (After this time interval, the 2Q system evolves freely.)

So, our task reduces to modeling \( \hat{V} \), so as to one may write:

\[ \exp\{-i\tau \hat{V} / \hbar\} = \hat{P}_1 z \otimes \hat{I}_2 + \hat{P}_2 z \otimes \hat{\sigma}_{2x}. \]  

(16)

4.1 A model of \( \hat{V} \)

Notice: the r.h.s. of (16) is diagonalizable (it is ”separable” [4]) in the noncorrelated basis \{\(|i\rangle_{1z}|j\rangle_{2x}, i, j = 0, 1\}. So, the same must apply to the l.h.s. of eq. (16).

The simplest form of \( \hat{V} \) which could fit this requirement is:

\[ \hat{V} = \hat{A}_1 \otimes \hat{B}_2, \]  

(17)

assuming that:

\[ 1z\langle i|\hat{A}_1|j\rangle_{1z} = A_i \delta_{ij} \]  

(18)

\[ 2x\langle m|\hat{B}_2|n\rangle_{2x} = B_m \delta_{mn} \]

and \(|m\rangle_{2x}\) represent the eigenstates of \( \hat{\sigma}_{2x} \).

Clearly, eq. (18) is equivalent with

\[ [\hat{A}_1, \hat{\sigma}_{1z}] = 0, \]  

(19)

\[ [\hat{B}_2, \hat{\sigma}_{2x}] = 0, \]

i.e. with

\[ \hat{A}_1 = \sum_i A_i |i\rangle_{1z} \langle i|_{1z}, \]

(20)

\[ \hat{B}_2 = \sum_m B_m |m\rangle_{2x} \langle m|_{2x} \]

Now, we should choose \( A_i \)s and \( B_m \)s, so as to satisfy eq. (16).

4.2 A model of \( \hat{A}_1 \) and \( \hat{B}_2 \)
Bearing in mind eq. (20), the l.h.s. of eq. (16) - cf. [ ] - reads:

$$\exp\{-i\tau\hat{V}/\hbar\} = \hat{P}_{1z} \otimes \exp\{-i\tau A_1 \hat{B}_2/\hbar\} + \hat{P}_{2z} \otimes \exp\{-i\tau A_2 \hat{B}_2/\hbar\}. \quad (21)$$

When compared to eq. (16), it leads to:

$$\exp\{-i\tau A_1 \hat{B}_2/\hbar\} = \hat{I}_2 \quad (22a)$$

$$\exp\{-i\tau A_2 \hat{B}_2/\hbar\} = \hat{\sigma}_{2x} \quad (22b)$$

The choice $A_1 = 0$ is obvious.

On the other side, eq. (20) suggests that the l.h.s. of (22b) - cf. [4] - can be written as

$$\exp\{-i\tau A_2 B_1/\hbar\} \hat{\pi}_{1x} + \exp\{-i\tau A_2 B_2/\hbar\} \hat{\pi}_{2x}, \quad (23a)$$

while the r.h.s. reads:

$$\hat{\pi}_{1x} - \hat{\pi}_{2x}. \quad (23b)$$

Equating (23a) and (23b) it follows that

$$\exp\{-i\tau A_2 B_1/\hbar\} = 1, \quad (24)$$

$$\exp\{-i\tau A_2 B_2/\hbar\} = -1, \quad (25)$$

which directly implies:

$$B_1 = \frac{nh}{\tau A_2}, \quad B_2 = \frac{(2m+1)\hbar}{2\tau A_2}. \quad (26)$$

### 4.3 A model of $\hat{V}$

So one obtains:

$$\hat{V} = \hat{P}_{2z} \otimes [(nh/\tau)\hat{\pi}_{1x} + ((2m+1)\hbar/2\tau)\hat{\pi}_{2x}], \quad (27)$$

for mutually independent integers, $m, n$, and $\tau$ fixed.

Now one may wonder if, for fixed $\tau$, the interaction may diverge from the exact duration $\tau$. But this does not make any particular problem. Let us suppose that the real interaction duration equals $\tau' = \tau \pm \epsilon, \epsilon \ll \tau$. Then eq. (15) reads:

$$\hat{V}' = \exp\{-i(\tau'/\hbar\tau)\hat{P}_{2z} \otimes [nh\hat{\pi}_{1x} + ((2m+1)\hbar/2\tau)\hat{\pi}_{2x}]\} = \hat{U}(t) \cdot \hat{u}(t), \quad (28)$$

where

$$\hat{u}(t) = \exp\{i(\epsilon/\hbar\tau)\hat{P}_{2z} \otimes [nh\hat{\pi}_{1x} + ((2m+1)\hbar/2\tau)\hat{\pi}_{2x}]\}, \quad (29)$$

and, obviously: $\hat{u}(t) = \hat{I} + O(\epsilon/\tau)$. So, $\hat{V}$ and $\hat{V}'$ satisfy the approximation criterion [1]: $\hat{V} - \hat{V}' \sim O(\epsilon/\tau)$.  


4.4 The Toffoli gate

In full analogy one may obtain the quantum-mechanical model of the Toffoli gate. But this will be omitted here.

5. The symmetry considerations

Here we pose the question of the symmetry group of the interaction eq. (27). A bit of care is required with this regard: whilst the states \{\ket{i}\} of both the qubits can physically be virtually arbitrary (e.g., the ”ground”, \ket{g}, and ”excited”, \ket{e}) states, all the considerations are formally equivalent with a spin-1/2 system. It particularly means that the actual Hilbert space(s) reduces to a 2-dimensional space, and the corresponding algebra is the well known SU(2) algebra. And this notion points out the symmetry groups that should be considered.

As with the spin-1/2 system, the transformations to be considered reduce to the next two unitary groups:

(i) the qubits’ exchange (the permutation group), and
(ii) the global rotations of the two-spin-1/2 system.

I.e., we assume that all the other transformations (from the Galilei, or Poincare group) are not defined.

By the very definition (cf. Section 2), the CNOT transformation clearly distinguishes between the two qubits: the ”the first qubit” is usually referred to as the ”controlled qubit”, while the ”the second qubit” is usually referred to as the ”target qubit”. No exchange of the qubits is allowable.

So, it remains to consider the rotations.

As it is well known, the global rotations are generated by the elements, \hat{S}_n (a projection of spin along \vec{n}), of the SU(2) algebra:

\[ \hat{S}_n = \hat{S}_{1n} + \hat{S}_{2n}. \]  

That is, the global rotation about an axis \vec{n} by the angle \theta reads:

\[ \hat{R}_{\vec{n}} = \exp(-i\hat{S}_n \theta / \hbar). \]  

But this operator can always be written in the (obviously separable \cite{4}) form:

\[ \hat{R}_{\vec{n}} = \hat{R}_{\vec{n}}^{(1)} \otimes \hat{R}_{\vec{n}}^{(2)}, \]  

where

\[ \hat{R}_{\vec{n}}^{(i)} = \exp(-i\hat{S}_{in} \theta / \hbar). \]

So, for eq. (27), the global-rotations-symmetry-requirement implies (as it can be easily seen):

\[ [\hat{S}_{1n}, \hat{\sigma}_{1z}] = 0, \]  

\[ [\hat{S}_{2n}, \hat{\sigma}_{2x}] = 0. \]
However, and this is the point to be emphasized, this cannot be fulfilled; at least not without changing the definition eq. (3) (cf. Section 6).

This notion follows from the isomorphism between the Hilbert spaces of the two qubits. Particularly, the isomorphism implies equivalence of eqs. (34a,b) with:

\[ \hat{S}_{in}, \hat{\sigma}_{iz} = 0, \quad (35a) \]

\[ \hat{S}_{in}, \hat{\sigma}_{ix} = 0, \quad (35b) \]

for both \( i = 1, 2 \) - which certainly cannot be fulfilled for the qubits. So we conclude that \( \hat{H}_{int} \) does not have any global symmetry!

5.1 The isolated systems

Throughout this paper we examine (cf. Introduction) the two-qubit system as an isolated quantum system.

To this end, for an isolated quantum ("microscopic") system it is practically a matter of principle that its Hamiltonian has at least one group of the global symmetry. [E.g., for an EPR pair, there is the full (e.g., rotational) symmetry of the "pair". In the collision processes it is both theoretically and experimentally verified the perfect energy (momentum) conservation. The same applies to the radiative processes; just remind the unsuccessful trial [5] in establishing the oposite.]

However, in Section 4 we have considered the two-qubit system as an isolated system, but we have obtained that \( \hat{H}_{int} \) does not have any global symmetry - which, also, directly follows from eq. (5). This produces a contradiction.

5.2 The contradiction

It is worth emphasizing the above distinguished contradiction.

Physically, it is practically a matter of principle to deal with a global-symmetry group of the Hamiltonian of an isolated quantum system.

But, as regards the CNOT transformation, such a group does not exist.

5.3 More general transformations

In order to find a "symmetry group" of \( \hat{H}_{int} \), eq. (27), one could look for the more general transformations. Certainly, this "search" reduces to looking for the hermite-conjugate "generators" of the "symmetry" transformations which would commute with \( \hat{H}_{int} \).

Then one may show that the "generators" of the nontrivial transformations appear as the linear combinations of the next operators:

\[ \hat{I}_1 \otimes \hat{\sigma}_{2z}, \quad \hat{\sigma}_{1z} \otimes \hat{I}_2, \quad \hat{\sigma}_{1z} \otimes \hat{\sigma}_{2x}. \quad (36) \]

But the corresponding transformations have no physical interpretation in terms of the global transformations of the 2Q system.

So, there remains the above conclusion: \( \hat{H}_{int} \) does not have any global symmetry.

6. A proposal for removing the contradiction
The contradiction can be “easily” removed by abandoning the initial assumption - that the 2Q system is isolated.

Without details, the idea for overcoming the contradiction is as follows: To consider the 2Q system as an open system, each qubit separately interacting with a ”mediator”, i.e., with an external system whose interactions with the qubits, effectively, lead to the change of the states of 2Q system, as defined by \( U_{CNOT} \).

Certainly, then \( U_{CNOT} \) requires re-interpretation: it does not refer to an isolated quantum system, but it represents a net effect of interaction of the qubits with a ”mediator”, which mediates the qubits’ mutual ”interaction”. Finally, since the 2Q system is an open system, its dynamics is neither unitary, nor unique [6], and the net-effect-\( U_{CNOT} \) follows after ignoring the states of the ”mediator”, \( M \).

A REMARK: It is important to note that the paradox can be also removed by redefining the definition, eq. (3) in either of the two ways: (i) by redefining the states of, e.g., the first qubit: instead the eigenstates of \( \hat{\sigma}_{1z} \), one could consider the eigenstates of \( \hat{\sigma}_{1x} \), which would lead to:

\[
\hat{U}_{CNOT} = \hat{P}_1 \otimes \mathbb{I}_2 + \hat{P}_2 \otimes \hat{\sigma}_{2x},
\]

(37)

with obvious symmetry (rotation about \( x \)-axis), and/or (ii) relativizing the isomorphism between the Hilbert state spaces of the qubits: e.g., by considering the mutually nonidentical qubits; then eqs. (35a,b) need not to follow from eqs. (34a,b), for the isomorphism bears ambiguity, thus reducing the problem onto the above point ””(i)”.

Still, with this regard appear further problems: Whether the redefinitions can be successfully implemented for an array of \( n \gg 1 \) the qubits, especially with regard to the necessity of the different preparations of the states of the qubits, in practice. Finally, both proposals bear ambiguities (concerning the definitions of the qubits’ states, and concerning the isomorphism), which open the question, e.g., why would one deal with eq. (37), instead of with eq. (5)?

So, we conclude that the above remark, i.e. necessity of mediating the interaction between the qubits, proves physically a favourable solution of the paradox, really overcoming the above mentioned ambiguities.

7. Conclusion

The CNOT transformation of the two-qubit system, considered as an isolated quantum system, cannot be justified. For it implies nonexistence of any global symmetry for the isolated two-qubit system.

We propose to extend this system by a ”mediator”, \( M \), so as to the whole, \( 1 + 2 + M \) evolves unitary in time, but so that when ignoring the state(s) of \( M \), as the net effect of the evolution appears the CNOT transformation. This proposal will be elaborated elsewhere.

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