Promoting quantum correlations in DQC1 model via post-selection

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The deterministic quantum computation with one qubit (DQC1) model is a restricted model of quantum computing able to calculate efficiently the normalized trace of a unitary matrix. In this work we analyse the quantum correlations named entanglement, Bell’s nonlocality, quantum discord, and coherence generated by the DQC1 circuit considering only two qubits (auxiliary and control). For the standard DQC1 model only quantum discord and coherence appear. By introducing a filter in the circuit we purify the auxiliary qubit taking it out from the totally mixed state and consequently promoting other quantum correlations between the qubits, such as entanglement and Bell’s nonlocality. Through the optimization of the purification process we conclude that even a small purification is enough to generate entanglement and Bell’s nonlocality. We obtain, in average, that applying the purification process repeatedly by twelve times the auxiliary qubit becomes 99% pure. In this situation, almost maximally entangled states are achieved, which by its turn, almost maximally violate the Bell’s inequality. This result suggests that with a simple modification the DQC1 model can be promoted to a universal model of quantum computing.

I. INTRODUCTION

As quantum correlations are exclusive to the quantum realm, we may expect that advantages to process, store, and transmit information are somehow connected to them. In the case of processing information, to have a speedup in relation to classical algorithms, quantum computing with pure states requires entanglement. However, this requirement is not clear for quantum computation with mixed states. For instance, the Deterministic Quantum Computation with One Qubit (DQC1) model only quantum discord and coherence appear. By introducing a filter in the circuit we purify the auxiliary qubit taking it out from the totally mixed state and consequently promoting other quantum correlations between the qubits, such as entanglement and Bell’s nonlocality. Through the optimization of the purification process we conclude that even a small purification is enough to generate entanglement and Bell’s nonlocality. We obtain, in average, that applying the purification process repeatedly by twelve times the auxiliary qubit becomes 99% pure. In this situation, almost maximally entangled states are achieved, which by its turn, almost maximally violate the Bell’s inequality. This result suggests that with a simple modification the DQC1 model can be promoted to a universal model of quantum computing.

II. QUANTUM CORRELATIONS IN THE STANDARD DQC1 MODEL

Introduced in 1998 by Knill and Laflamme, the Deterministic Quantum Computation with One Qubit (DQC1) is a computing model that evaluates the normalized trace of any unitary operator using a measurement in a single qubit. The DQC1 circuit (see Fig. 1) consists of a control qubit in the state

\[ \rho_0(\alpha) = \frac{(I + \alpha \sigma_Z)}{2}, \]

where \( \sigma_Z \) is the Pauli matrix \( Z \), a certain degree of coherence controlled by \( \alpha \) (0 \( \leq \alpha \leq 1 \)), and \( n \) auxiliary qubits initially in the totally mixed state

\[ \rho_n = \frac{I^{\otimes n}}{2^n}, \]

where \( I \) the identity operator.

Besides the Hadamard gates,

\[ H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \]

applied on the first qubit, the computation is performed by a controlled unitary between the first and auxiliary qubits. The result is obtained by measuring the expected values of the operators associated to the control qubit, whose precision is independent on the dimension of the unitary transformation \( U_n \) and depends only on the number of runs of the quantum circuit. In contrast, the simplest classical algorithm to calculate the trace of a matrix depends on its dimension, which one can increase exponentially according to number of qubits in the system.

With this advantage in mind, the idea is to map certain problems into DQC1 model. Despite of not being
a universal model of quantum computing, some quantum solutions obtained through this model present advantages in comparison to their classical counterparts, such as spectral density estimation \[3\], testing integrability \[11\], Shor factorization \[12\], evaluation of average fidelity decay \[13\], estimate of Jones Polynomials \[14\], and quantum metrology \[15\] \[16\]. Inspired by these results, some experimental implementations of this model have been made in optical \[17\] \[18\], Nuclear Magnetic Resonance \[19\] \[20\], superconducting materials \[21\], and cold atoms \[22\].

A. Quantum Correlations in DQC1 model

We start by writing the output state of the DQC1 circuit for two qubits in the Fano representation \[23\],

\[
\rho = \frac{1}{4} \left[ I_A \otimes I_B + I_A \otimes \left( \vec{r} \cdot \vec{\sigma}^B \right) \right.
+ \left( \vec{s} \cdot \vec{\sigma}^A \right) \otimes I_B + \sum_{i,j=x,y,z} c_{ij} \sigma_i^A \otimes \sigma_j^B \right],
\]

(1)

where the polarization vectors are \( \vec{r} = tr[\rho (I_A \otimes \sigma^B)] \) and \( \vec{s} = tr[\rho (\vec{\sigma}^A \otimes I_B)] \), the elements of the correlation matrix \( C = c_{ij} = tr[\rho (\sigma_i^A \otimes \sigma_j^B)] \), the indices \( A \) and \( B \) refer to the first and second subsystems, and \( i,j = x,y,z \) to the indices of a vector of Pauli matrices, namely \( \{ \sigma_x, \sigma_y, \sigma_z \} \).

It is simple to define the quantum correlations used throughout this work (Bell’s nonlocality, entanglement, quantum discord, and coherence) using this representation.

Bell’s nonlocality - The Bell’s inequality can be evaluated by the quantity \[24\],

\[
B(\rho) = 2\sqrt{m_1 + m_2},
\]

(2)

where \( m_1 \) and \( m_2 \) are the two largest eigenvalues of the matrix \( T = CC^T \), where \( T \) means the transposition operation. If \( B(\rho) \leq 2 \) the Bell’s inequality is not violated, otherwise, non-local effects might appear. The values of \( B(\rho) \) are comprised in the interval \([0, 2\sqrt{2}]\), with the maximum violation being achieved by the entangled pure states, such as the Bell entangled states.

Entanglement - To quantify bipartite entanglement, we used Negativity \[25\] defined as

\[
N(\rho) = \frac{\|\rho^{T_A}\|_1 - 1}{2},
\]

(3)

where \( T_A \) is the partial transposition of the subsystem \( A \) and \( \| \cdot \|_1 \) is the trace norm. The negativity indicates how far the partial trace of the density matrix is far from positive, and consequently, how much entangled the subsystems are. For a two-qubit system \( N(\rho) \in [0, 1/2] \).

Quantum discord - The geometric discord of an arbitrary two-qubit state is \[27\],

\[
D(\rho) = \frac{1}{4} \left( \| \vec{s} \|_2^2 + \| C \|_2^2 - \lambda_{\text{max}} \right),
\]

(4)

where the norms in the right hand side of the equation above have been calculated using the euclidean (for vector \( \vec{s} \)) and Hilbert-Schmidt (for matrix \( C \)) norms. \( \lambda_{\text{max}} \) represents the largest eigenvalue of the matrix

\[
\Lambda = \vec{s} \cdot \vec{s}^T + CC^T.
\]

The values of quantum discord are restricted to the interval \( D(\rho) \in [0, 1/2] \).

Coherence - The trace norm Coherence is measured using \[26\] \[27\],

\[
C(\rho) = \| \rho - \rho_{\text{diag}} \|_1,
\]

(5)

where \( \rho_{\text{diag}} \) denotes the state obtained from \( \rho \) using just the diagonal elements. Basically, this measure sums the absolute values of all off-diagonal terms of \( \rho \) so that \( C(\rho) \in [0, 3] \) for a two-qubit system.

To explore the quantum correlations presented in the output states of the DQC1 circuit for two qubits (see Fig. 1), we chose \( 10^6 \) random initial qubit states according to Hilbert-Schmidt measure \[28\] and also \( 10^6 \) unitary matrices \( (U_1) \) from Haar measure \[29\] \[30\]. The quantum correlations generated between the two qubits at the end of the circuit are shown in Fig. 2 where each dot is obtained for a given final density matrix.

As it is already known, there is no entanglement between the control and the auxiliary qubits in the standard DQC1 model \[4\], and a straightforward consequence of this is no violation of Bell’s inequality, as shown in Figs. 2a and 2b. Superposition (quantified by coherence) is vital for the appearance of others correlations as shown in Figs. 2a and 2c. We also have, Fig. 2c showing states with non vanishing quantum discord \( D(\rho) \) and coherence, confirming they are intimately related. Note the maximum values achieved by coherence and quantum discord, \( C_{\text{max}}(\rho) = 1 \) and \( D_{\text{max}}(\rho) = 0.1244 \), respectively. They are far from reaching the maximum values accessible for general two qubit states, i.e., 3 and 0.5, respectively.

III. POST-SELECTION IN DQC1 MODEL

Inspired by Ref. \[12\], we analyzed the effect of the post-selection on promoting quantum correlations in the DQC1 model for two qubits.
in order to purify the auxiliary qubit, we post-select for
of Bell’s inequality emerge in this system [32]. Thus,
an appropriate unitary
A state different from the maximum mixture, then, for
just one component of the state survives.
(Ua, η) = \begin{bmatrix} 0 & 1 \\ 0 & η \end{bmatrix} U_a^†, (6)
with η ∈ [0, 1] and U_a is a unitary matrix. η represents
the probability of success of acting this filter considering
the complete measurement \{F(Ua, η), I − F(Ua, η)\}. For
the particular case η = 1, the filter reduces to the identity
operator, doing nothing on the control qubit, while, for
η < 1, it diminishes the contribution coming from one
component of the state in the direction determined by
the unitary transformation U_a. In the limit case η = 0,
just one component of the state survives.

As it is well known, if the auxiliary qubit starts in
a state different from the maximum mixture, then, for
an appropriate unitary U_1, entanglement and violation
of Bell’s inequality emerge in this system [32]. Thus,
in order to purify the auxiliary qubit, we post-select for
certain values of η and investigate the role played by this
filter parameter on the quantum correlations between the
qubits.

A. Benchmarking the DQC1 with post-selection

To proceed with this investigation, we used a DQC1
with post-selection, see Fig. 3. The state before filtering
is
\[ ρ_{0f} = (H ⊗ I)U(H ⊗ I)ρ_0(H ⊗ I)U^†(H ⊗ I), \] (7)
and the final state is
\[ ρ_f(U_a, η) = \frac{F(U_a, η)ρ_{0f}F(U_a, η)^†}{\text{tr}[F(U_a, η)ρ_{0f}F(U_a, η)^†]} \] (8)
for some choice of η ∈ [0, 1] and unitary matrix U_a.

Following [33], we first analyze the fidelity,
\[ F(ρ_1, ρ_2) = \left( \sqrt{F(ρ_1, ρ_2)\sqrt{ρ_1^†}} \right)^2, \]
between 10^4 pairs of output states ρ_f and ρ_f′, choosing
an initial pure state ρ_0 for the control qubit drawn from
Hilbert-Schmidt measure, a controlled unitary gate U_1,
and a unitary U_a drawn from Haar measure and fixed
values of η ∈ {0, 1/2, 1}.

The probability distributions of F(ρ_f, ρ_f′) in Fig. 4
shows the average fidelity between ρ_f and ρ_f′ diminishing
as η → 0. We can see it as a numerical evidence
that the DQC1 with post-selection distributes the states
more distantly (according to the Bures metric [34]), and
also with more accessible states in the two-qubit Hilbert
space, which will be clear when we present the promotion
of quantum correlations further in this article.

To understand qualitatively this result let us remember
that the motivation of the DQC1 model relies on Nuclear
Magnetic Resonance systems, whose two-qubit density
matrices have the form
\[ ρ_{NMR} = \frac{1 − \epsilon}{4} I_{4×4} + \epsilon |ψ⟩⟨ψ|, \] (9)
with 0 ≤ ϵ ≤ 1 and I_{4×4} and |ψ⟩ are the identity operator
and a pure state in the two-qubit Hilbert space. If we
calculate the fidelity for states of the form ρ_{NMR} it is easy
to verify that for small values of ϵ states with fidelities
closer to one are more frequent, which is similar to the
standard DQC1 model.
FIG. 4. Empirical probability distribution of the fidelity between $10^4$ randomly chosen $\rho_f$ and $\rho'_f$ after the DQC1 with post-selection (see Eq. 8) for fixed values of $\eta \in \{0, 1/2, 1\}$.

B. Purity and quantum correlations in DQC1 model

As mentioned before, the purity $P(\rho) = \text{tr} \rho^2$ of the auxiliary qubit also determines the possibility of promoting quantum correlations in DQC1 model. The purity varies from $P(\rho) = 1/2$ for a totally mixed qubit state to $P(\rho) = 1$ for a pure qubit state. In Fig. 5 we run the same protocol above and take the average maximum value of the purity for a specific value of $\eta$. We observe that the average maximum value of the purity is approximately $P(\rho) \simeq 0.62$ for $\eta = 0.5$ and as $\eta$ approaches 1 the purity converges to its minimum value, as expected, since for $\eta = 1$ the filter has no effect on the auxiliary qubit.

FIG. 5. Purity as function of the probability of success $\eta$ for DQC1 model with two qubits and post-selection. Each dot represents the average maximum value of the achieved purity for the auxiliary qubit with a specific $\eta$.

FIG. 6. Normalized quantum correlations as function of purity $P(\rho)$. Each dot represents the average maximum value of the quantum correlations for a given purity.

To estimate the number of states that have been promoted after the post-selection process, i.e., the number of states whose quantum correlations increased after the filtering procedure, we analyse the density of states. The density of states is defined as the ratio between the number of states after the post-selection process with a correlation value greater than the maximum value of the correlation achieved by the states in the standard DQC1 model (without post-selection). The maximum values of quantum discord, quantum coherence, and $B(\rho)$ attained by the standard DQC1 circuit (see Fig. 2) are 0.1244, 0.9992, and 1.9974, respectively. Figure 7 presents density of states for quantum discord (green discs), quantum coherence (orange diamonds), and $B(\rho)$ (black stars) for the different values of $\eta$ considering a total of $10^4$ states. As there is no entanglement between the control and the auxiliary qubit in the standard DQC1 model, the density of states defined above does not apply for this correlation. We observe that the higher the $\eta$ the lower the density of states that overcome the value of these correlations for DQC1 model without post-selection. This reinforce the strong connection between the mixedness of the auxiliary qubits and the quantum correlations in the model. As in the standard DQC1 model the maximum value achieved by $B(\rho)$ is approximately 2, all states used...
to build Fig. 7 (black stars) violate the Bell’s inequality. These plots give us information about the number of states that are accessible after the post-selection process, which ones constitute a resource for quantum computation.

We noticed it was necessary 12 steps on average to achieve the desired value of purity. The relation between the quantum correlations with the steps of purification are shown in Figures 8-13. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and initial states of the control qubit used to compute the quantum correlations for each purification step of the auxiliary qubit. In order to keep the figures legible, we have plotted only 5 steps of a total of 12, i.e., the first, second, third, fourth, and twelfth ones. The blue surfaces represent the mean value of quantum correlations after the first step of purification, while the green ones after the last step of purification, in which the auxiliary qubit achieves $P(\rho) = 0.99$.

C. Purification optimization

Now we want to find optimal strategies of filtering, without fixing the parameter $\eta$, to reach a purity of $P(\rho) = 0.99$ for the auxiliary system.

For this optimization, we chose the following procedure:

1. The initial pure state $\rho_0$ for the control qubit and the controlled unitary gate $U_1$ are drawn from Hilbert-Schmidt and Haar measures, respectively.

2. The parameters of the filter $F$, which include $\eta$ and the unitary $U_a$, are chosen such that

$$\arg\min_{\eta,U_a} \{P(\text{tr}_c[\rho_f(U_a, \eta)])\},$$

where $\text{tr}_c[\rho_f(U_a, \eta)]$ is the state of the auxiliary system after the post-selection, tracing the control system out.

3. If $P(\text{tr}_c[\rho_f(U_a, \eta)]) \approx 0.99$ we stop.

4. Otherwise, the purified state of the auxiliary qubit is chosen in the DQC1 circuit instead of the identity and we optimize again for the same choice of initial pure state $\rho_0$ for the control qubit and the controlled unitary gate $U_1$.

![Figure 7](image_url) Density of states, defined as the ratio between the number of states after the post-selection process with a correlation value greater than the maximum value of the correlation achieved by the states in the standard DQC1 model (without post-selection), versus the probability of success $\eta$ of the purification protocol. The total number of states analyzed for each correlation is $10^4$.

![Figure 8](image_url) Quantum discord $D(\rho)$ versus $B(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

Figures 8-10 agree for highly purified auxiliary states once quantum discord and entanglement quantify the same kind of correlation [7].

In Fig. 10 we observe that in all steps of purification of the auxiliary qubit, the states have non-null coherence, achieving the maximum value of approximately 1.5. Such a value is also achieved by states that violate almost maximally the Bell’s inequality, i.e., they are of the form $(|00\rangle + |11\rangle)/\sqrt{2}$, which gives us a coherence value of $\sqrt{2} \approx 1.41$.

Figures 11 and 12 show that for the last step of purification, almost all states have $C(\rho) > 1$, which demonstrate the efficiency of the purification protocol.

The general behavior of quantum correlations pre-
FIG. 9. Negativity $N(\rho)$ versus $B(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

FIG. 10. Quantum coherence $C(\rho)$ versus $B(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

FIG. 11. Quantum discord $D(\rho)$ versus quantum coherence $C(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

FIG. 12. Quantum coherence $C(\rho)$ versus negativity $N(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

FIG. 13. Agrees with the result presented in Ref. 35, which one states that when using 2-norm, quantum discord is lower bounded by negativity. As mentioned above, for entangled states almost pure, both measures become quite similar.

IV. CONCLUSIONS

In this work we showed how to promote quantum correlations, such as coherence, quantum discord, entanglement, and Bell’s nonlocality, present in the output state of the DQC1 model for two qubits. As already known, in the standard DQC1 model for two qubits there are only quantum discord and coherence. By applying a filtering process combined to optimization protocols, entanglement and Bell’s nonlocality arise in this system, even for a small purification of the auxiliary qubit. In the case we reintroduced the purified auxiliary qubit into the circuit again, we observed that the number of purification steps that are needed to achieve a maximum purity of 0.99 is on average 12 steps. For this level of purity the qubits become practically maximally entangled and violate the Bell’s inequality almost maximally too. Our results suggest that it is possible to promote this restricted model of quantum computing to a universal one by using post-selection with a specific filter, although a
FIG. 13. Quantum discord $D(\rho)$ versus negativity $N(\rho)$. Each surface with different color shows the mean value of $10^4$ random unitary matrices $U_1$ and control qubit initial states used to compute the quantum correlations for each purification step of the auxiliary qubit. Due to the similar behavior of the quantum correlations for the intermediate steps of the purification process only five of a total of twelve steps have been plotted.

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