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Correlations in the Grover search

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Abstract

The Grover search is a well-known quantum algorithm that outperforms any classical search algorithm. It is known that quantum correlations such as entanglement are responsible for the power of some quantum information protocols. But entanglement is not the only kind of quantum correlations. Other quantum correlations such as quantum discord are also useful to capture some important properties of the nonclassical correlation. Also there is no well-accepted and clear distinction between quantum correlations and classical correlations. In this paper, we systematically investigate several kinds of correlations including both quantum and classical in the whole process of the Grover search algorithm. These correlations are the concurrence, entanglement of formation, quantum discord, classical correlation and mutual information. The behaviors of quantum discord, classical correlation and mutual information are almost the same while the concurrence is different in the qubit–qubit case. For the qubit partition $1 : n$ case, the behaviors of all correlations are qualitative the same. When the search is over, all kinds of correlations are zero, we argue that this is necessary for the final step in the search.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

It is known that quantum computing has great advantages over classical ones by several quantum algorithms, e.g. the Grover search algorithm [1] and Shor algorithm [2]. The Grover search algorithm provides a quadratic temporal speedup over the best classical search algorithm when they both require the same spatial resources to perform the same search task. It is believed that the outstanding performance of a quantum computer comes from the quantum phenomena such as quantum correlations, superposition, interference, etc in its resources qubits. Quantum correlation, especially entanglement, is one of the crucial issues in quantum information theory and has been studied extensively [3]. It is clear that quantum entanglement is essential in such tasks like quantum teleportation [4], superdense coding [5], entanglement assisted classical capacity of the quantum channel [6], etc. It is also believed that quantum entanglement is necessary for the Grover search [1] and the Shor algorithm [2] though the role of entanglement is not as clear as for other quantum information tasks like teleportation. Some properties of entanglement in the Grover search have been studied [7–9]. On the other hand, quantum entanglement may not be necessary for a model of quantum information processing introduced by Knill and Laflamme in [10]. Still such a device can outperform its classical counterpart. Thus, other quantum correlations different from entanglement are necessary in describing such a model. Ollivier and Zurek have recently defined the quantum discord to measure the quantum correlations [11]. Datta *et al* then applied quantum discord to characterize the correlations present in the model introduced in [10]. They found that while there is no entanglement between the control qubit and the mixed ones, the quantum discord across this split is nonzero, see [12]. Recently Lanyon *et al* implemented the above model in an all-optical architecture, and experimentally observed the generated correlations, see [13].

Motivated by the above fact that in certain algorithms some kinds of correlations such as quantum discord but not entanglement play a fundamental role, we want to know whether this is true for the Grover search algorithm, by studying several well-known correlations as well as entanglement in the process of search. In this paper, we consider a quantum register consisting of n qubits. We adopt concurrence as an entanglement measure and use quantum discord, classical correlation and mutual information to quantify correlation. To calculate entanglement or correlations, we have to identify two subsystems, where two different methods are used. (i) One method is that naturally we divide n qubits into two subsystems consisting of k and $n-k$ qubits, respectively. (ii) The other is that we calculate a two-qubit reduced density matrix and each subsystem only contains one qubit.

When we use method (i) to divide the whole system into two subsystems, we find that all correlations, as well as entanglement, have qualitatively the same behaviors, see figures 6–9. This suggests that during the Grover search the correlations in pure state can be described well by any correlation measures, quantum or classical. But when method (ii) is used, namely in a two-qubit reduced state, the behaviors of correlations are different from that of entanglement quantified by concurrence. Concurrence still firstly increases to its maximum and then decreases to almost zero, but other measurements of correlations repeat that routine for a second time, see figures 2–5. We also find that the increasing rate of success probability behaves the same way just as the concurrence does. The concurrence and the increasing rate of success probability get their maximal values almost at the same time. Entanglement measured by concurrence acts as an indicator of the increasing rate of success probability in Grover search. This suggests that in the Grover search algorithm the place of entanglement cannot be replaced by other correlations. The power of the Grover search depends on the ability to firstly increase the entanglement and then eliminate it.

The paper is organized as follows. In section 2, we briefly review the Grover search algorithm. In section 3, we introduce entanglement and different kinds of correlations which will be used in this paper including the mutual information, classical information and quantum discord. In section 4, we calculate the evolutions of the above correlations during the Grover search and show the results in several figures. These results are analyzed in section 5 and summarized in section 6.

2. Review of Grover search

We briefly review the standard Grover search algorithm [1, 14]. Suppose we have n-qubit register constructing a database of dimension $N = 2^n$. They are initialized

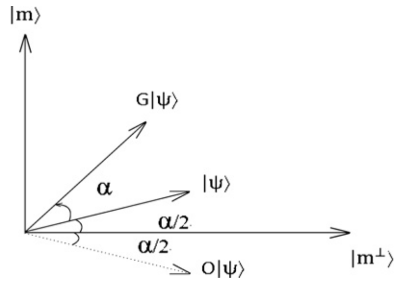

Figure 1. This figure shows the role of iteration played in the Grover search. $G = (2|\psi\rangle\langle\psi| - I)O$. Firstly, O reflects $|\psi\rangle$ according to $|m^\perp\rangle$. Then $(2|\psi\rangle\langle\psi| - I)$ reflects $O|\psi\rangle$ according to $|\psi\rangle$. We can check that $G|\psi\rangle + O|\psi\rangle = (G + O)|\psi\rangle = (2\langle\psi|O|\psi\rangle)|\psi\rangle$, and what in the bracket is a C number. Therefore, $|\psi\rangle$ is the axis of the reflection form $O|\psi\rangle$ to $G|\psi\rangle$. So one whole iteration turns the vector before iteration toward $|m\rangle$ by an angle α.

in the pure state $|0,\ldots,0\rangle$, and then subjected to local Hadamard gates, $H^{\otimes n}$, where $H = (|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|)/\sqrt{2}$. As a result the register is in an equal superposition pure state $|\psi\rangle = \frac{1}{N^{1/2}}\sum_{x=0}^{N-1}|x\rangle$. The Grover search algorithm requires repeated routine (called *iteration*), which can be expressed as $G = (2|\psi\rangle\langle\psi| - I)O$, where O is the oracle applied in the algorithm. If the state is just the target state to search, the oracle changes the phase of the state by π, i.e. $O|x\rangle = -|x\rangle$, when $|x\rangle$ is a state to search. If in contrast the state is not what we want, the oracle leaves it invariant.

The N states expressed by the n qubits are divided into two parts: the one belonging to the solution of the search, which is expressed as $\sum'|x\rangle$, and those which are not solutions to the search which are expressed as $\sum''|x\rangle$. The normalized states are defined as

$$|m\rangle = \frac{1}{\sqrt{j}}\sum_x{}'|x\rangle \tag{1}$$

$$|m^\perp\rangle = \frac{1}{\sqrt{N-j}}\sum_x{}''|x\rangle, \tag{2}$$

where j is the total number of the target states. The two states are orthogonal. For a simple case there is only one target state, i.e. $j = 1$. That is the case considered in this paper. It is easy to see that the initial equal superposition state can be expressed in the $|m^\perp\rangle$ and $|m\rangle$ bases as

$$|\psi\rangle = \sqrt{\frac{j}{N}}|m\rangle + \sqrt{\frac{N-j}{N}}|m^\perp\rangle. \tag{3}$$

Next, we check the effect of the iteration. We set the two orthonormal states $|m^\perp\rangle$ and $|m\rangle$ as two axes of a rectangular coordinate system. The initial equal superposition state $|\psi\rangle$ is a vector in the coordinate system. The oracle operator reflects the vector $|\psi\rangle$ according to $|m^\perp\rangle$. After that, the operator $2|\psi\rangle\langle\psi| - I$ reflects the vector $O|\psi\rangle$ according to $|\psi\rangle$. These two steps together realize turning the initial vector $|\psi\rangle$ toward the target vector $|m\rangle$ by an angle α, if the angle between the vector $|\psi\rangle$ and $|m^\perp\rangle$ is $\frac{1}{2}\alpha$, see figure 1. Simple calculations yield that $\alpha = \arccos\left(\frac{N-2j}{N}\right)$. Therefore, by repeating the above iteration routine the outcome state gets more and more closer to the target state. After r times of iterations the result states

$$|\psi_r\rangle = \sin\left(\frac{2r+1}{2}\alpha\right)|m\rangle + \cos\left(\frac{2r+1}{2}\alpha\right)|m^\perp\rangle. \tag{4}$$

The probability of success is

$$P = \sin^2\left(\frac{2r+1}{2}\alpha\right) \tag{5}$$

which is an important parameter in the Grover search. The best repeating times to get the biggest probability of success is

$$R = CI\left(\frac{\frac{\pi}{2} - \frac{\alpha}{2}}{\alpha}\right) \tag{6}$$

where $CI(x)$ denotes the integer closest to the real number x.

3. Quantum correlations

3.1. Entanglement

Entanglement is viewed as a key resource in quantum computing. It is believed to be responsible for the outstanding performances of quantum computers compared with their classical counterparts in many quantum information processing tasks, such as teleportation [4]. There are many measurements of entanglement defined from different considerations. Each measurement could capture certain aspects of entanglement, but none of these measurements is capable of involving all the features. Here we choose concurrence, a well-accepted entanglement measure, to investigate the behavior of entanglement in the whole process of the Grover search. Wootters has defined concurrence for the arbitrary state of two qubits in [15]. For a two-qubit state ρ, we can first calculate a relative matrix $\widetilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$, where σ_y is the Pauli matrix $\left(\begin{smallmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{smallmatrix}\right)$, and$\rho^*$ is the conjugation of ρ. Then the concurrence

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{7}$$

and $\lambda_i s$ are the square roots of the eigenvalues of the matrix $\rho\widetilde{\rho}$ in decreasing order, i.e. $\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4$. Fang *et al* have calculated the concurrence between any two qubits in the Grover search by Wootters' formula, see [16].

The above concurrence can be extended to the situation of a higher dimension pure bipartite state $|\psi\rangle$ [17–19]. We will use this form to study the entanglement of the Grover search. The concurrence of $|\psi\rangle$ is defined as

$$C(|\psi\rangle) = \sqrt{\frac{d}{d-1}\left(1 - \operatorname{Tr}\rho_r^2\right)}, \tag{8}$$

where ρ_r is the reduced density matrix obtained by tracing out one of the two subsystems, and d is the dimension of ρ_r. In this paper, we will calculate the concurrence between any k and the other $n-k$ qubits with this formula and will also show this result and other kinds of correlations in figures in the following.

3.2. Quantum discord

Quantum discord was first proposed by Ollivier and Zurek in [11] as the difference between two expressions of mutual information extended from the classical to quantum system. Datta *et al* used quantum discord to investigate a model which describes the power of one qubit, see [10, 12, 20]. In fact, the quantum discord that qualifies the quantum correlations can be viewed as the total correlation subtracting the classical correlation. One version of total correlation was defined by Groisman, Popescu and Winter in [21] in an operational way as the minimal amount of noise that is required to erase all the correlations between the two systems. They also showed that this definition of total correlation is equal to the quantum mutual information. Quantum correlation and classical correlation are generally involved together. To investigate correlations in the quantum algorithm, both classical and quantum correlations are useful to capture some properties of the correlation. Actually, when correlations, or other measurement data, are sufficient to guarantee the existence of a certain amount of quantum correlations in the system is a fundamental question in particular while concerning about the measurements [22].

In information theory, we know that the total correlation between two parties A and B is the mutual information denoted by $I(A, B)$, see for example [21]. For a quantum system

$$I(A, B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{9}$$

where $S(\rho)$ is the von Neumann entropy of ρ, $S(\rho) = -\mathrm{Tr}(\rho\log\rho)$, and $\rho_A(\rho_B)$ is the reduced density matrix of ρ_{AB} by tracing out $B(A)$.

Classical correlation between A and B was defined by Henderson and Vedral in [23, 24] as the maximum information we can get from A by measuring B. Before measuring B, the reduced density matrix of A is ρ_A. Then we choose a complete set of projectors $\{\Pi_i\}$ to measure the subsystem B, corresponding to the outcome i with the probability p_i. The state of A after the above measurement is $\rho_{A|i} = \frac{\mathrm{Tr}_B(\Pi_i\rho_{AB}\Pi_i)}{\mathrm{Tr}_{AB}(\Pi_i\rho_{AB}\Pi_i)}$, and $p_i = \mathrm{Tr}_{AB}(\Pi_i\rho_{AB}\Pi_i)$. So the information of A we can get by measuring B is $S(\rho_A) - \sum_i p_i S(\rho_{A|i})$. For a given density matrix ρ_{AB}, the above representation depends on the choice of measurement, i.e. we can obtain different results if we use different bases to apply the measurement. The classical correlation measures the biggest amount of information, that is

$$\begin{aligned} C(A, B) &= \max_{\{\Pi_i\}}\{S(\rho_A) - \sum_i p_i S(\rho_{A|i})\} \\ &= S(\rho_A) - \min_{\{\Pi_i\}} \sum_i p_i S(\rho_{A|i}). \end{aligned} \tag{10}$$

It can be checked easily that this definition of classical correlation satisfies several conditions. These conditions include (i) $C = 0$ for $\rho = \rho_A \otimes \rho_B$; (ii) C is invariant under local unitary transformations; (iii) C is non-increasing under local operations; (iv) $C = S(\rho_A) = S(\rho_B)$ for pure state, see [23].

Quantum discord expressed as D is the difference between the total correlation and the classical correlation, i.e.

$$\begin{aligned} D(A, B) &= I(A, B) - C(A, B) \\ &= \min_{\{\Pi_i\}} \sum_i p_i S(\rho_{A|i}) + (S(\rho_B) - S(\rho_{AB})). \end{aligned} \tag{11}$$

If we split the n-qubit system into one qubit slice and the other $n - 1$ qubits slice, and calculate the quantum discord between these two parts, we can obtain a computable result theoretically. That is because we can choose the one qubit slice as the part to be measured, and have the bases of measurement parameterized by θ and ϕ in the form of $\{\cos(\theta)|0\rangle + \mathrm{e}^{\mathrm{i}\phi}\sin\theta|1\rangle, \mathrm{e}^{-\mathrm{i}\phi}\sin\theta|0\rangle - \cos\theta|1\rangle\}$. Therefore, the minimum according to $\{\Pi_i\}$ in equation (11) has been changed into finding θ and ϕ to realize the minimum. In the next section, we will use this method to calculate the quantum discord between any one qubit and the other qubits .

4. Correlations in the Grover search

4.1. Density matrix for the total system and the two-qubit reduced density matrix

We have already known the form of the state after r times of $iterations$ in equation (4) in the $|m^{\perp}\rangle$ and $|m\rangle$ bases. The density matrix is

$$\begin{aligned}
\rho &= \sin^2\left(\frac{2r+1}{2}\alpha\right)|m\rangle\langle m| + \cos^2\left(\frac{2r+1}{2}\alpha\right)|m^{\perp}\rangle\langle m^{\perp}| \\
&\quad + \sin\left(\frac{2r+1}{2}\alpha\right)\cos\left(\frac{2r+1}{2}\alpha\right)(|m\rangle\langle m^{\perp}| + |m^{\perp}\rangle\langle m|) \\
&= \sin^2\left(\frac{2r+1}{2}\alpha\right)\frac{1}{j}\sum_{i,k}{}'|i\rangle\langle k| + \cos^2\left(\frac{2r+1}{2}\alpha\right)\frac{1}{N-j}\sum_{i,k}{}''|i\rangle\langle k| \\
&\quad + \sin\left(\frac{2r+1}{2}\alpha\right)\cos\left(\frac{2r+1}{2}\alpha\right)\frac{1}{\sqrt{j(N-j)}}\left(\sum_i{}'\sum_k{}''|i\rangle\langle k| + \sum_i{}'\sum_k{}''|k\rangle\langle i|\right) \\
&= a^2\frac{1}{j}\sum_{i,k}{}'|i\rangle\langle k| + b^2\frac{1}{N-j}\sum_{i,k}{}''|i\rangle\langle k| + ab\frac{1}{\sqrt{j}}\left(\sum_i{}'\sum_k{}''|i\rangle\langle k| + \sum_i{}'\sum_k{}''|k\rangle\langle i|\right)
\end{aligned} \tag{12}$$

where the $\sum'$ stands for the sum of all the states belonging to the search result, and the $\sum''$ means the sum of all the states that are not what to search, $a = \sin\left(\frac{2r+1}{2}\alpha\right)$ and $b = \frac{1}{\sqrt{N-j}}\cos\left(\frac{2r+1}{2}\alpha\right)$ are brought in to make the expression explicit. In the present work we study the simplest case of having only one target state, i.e. $j = 1$. Obviously, the above expression is in the computational bases, and its matrix form is

$$\begin{pmatrix}
a^2 & ab & ab & ab & ab & ab & ab & ab & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
ab & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & b^2 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}_{N\times N}. \tag{13}$$

We can get the two-qubit reduced density matrix from the above n-qubit one by tracing out any $n-2$ qubits. Mathematically the result can be obtained in the following way: the above $2^n \times 2^n$ matrix is first divided into $2^{n-2} \times 2^{n-2}$ parts symmetrically with every part of a 4×4 matrix. Now the initial matrix becomes a $2^{n-2} \times 2^{n-2}$ matrix whose every element is a 4×4 matrix. Then we sum the 2^{n-2} diagonal elements up to get a new 4×4 matrix,which is the reduced density matrix for any two qubits. It takes the following form:

$$\rho_2 = \begin{pmatrix}
a^2 + \left(\frac{N}{4}-1\right)b^2 & ab + \left(\frac{N}{4}-1\right)b^2 & ab + \left(\frac{N}{4}-1\right)b^2 & ab + \left(\frac{N}{4}-1\right)b^2 \\
ab + \left(\frac{N}{4}-1\right)b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2 \\
ab + \left(\frac{N}{4}-1\right)b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2 \\
ab + \left(\frac{N}{4}-1\right)b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2 & \frac{N}{4}b^2
\end{pmatrix}. \tag{14}$$

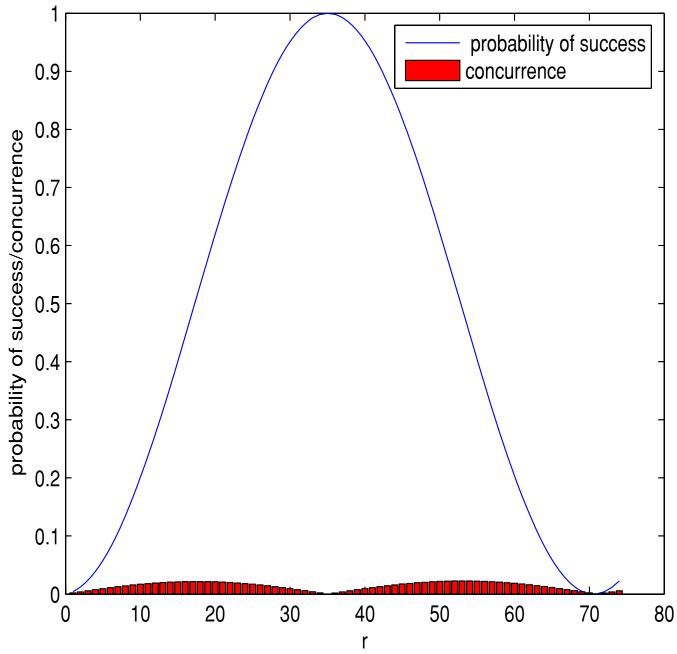

Figure 2. Concurrence between any two qubits for $N = 2048$ is obtained using formula (15) based on the reduced density matrix ρ_2 in equation (14). Similar result was first obtained in [16] where $N = 256$.

4.2. Concurrence and other kinds of correlations in the Grover search

Based on this reduced density matrix, Fang *et al* [16] used Wootters' formula mentioned above in equation (7) and calculated the concurrence between any two qubit sites as follows:

$$C_{1,1} = 2\left|\cos(\theta_0 - r\alpha) - \frac{1}{\sqrt{N-1}}\sin(\theta_0 - r\alpha)\right| \times \frac{1}{\sqrt{N-1}}\sin(\theta_0 - r\alpha). \tag{15}$$

This is the analytic pairwise entanglement in the Grover search. The evolution of the pairwise entanglement in the Grover search algorithm is calculated numerically and the result is shown in figure 2 compared with the probability of success in the search algorithm.

We can also use the two-qubit reduced density matrix (14) to calculate the mutual information, classical correlation and quantum discord between any two qubits. We first calculate the mutual information using equation (9). The numerical results are presented in figure 3. In the calculation, ρ_{AB} takes ρ_2, and $\rho_A = \rho_B$ is the reduced density matrix by tracing out one qubit from ρ_2.

Next, we will compute numerically the classical correlation according to equation (10). Still $\rho_{AB} = \rho_2$ in equation (14) and $\rho_A = \rho_B$ is the one-qubit reduced density matrix. The main task in this calculation is to find the minimum entropy of one qubit after the measurement on another. The measurement bases are parameterized by θ and ϕ in the form $\{\cos(\theta)|0\rangle + \mathrm{e}^{\mathrm{i}\phi}\sin\theta|1\rangle, \mathrm{e}^{-\mathrm{i}\phi}\sin\theta|0\rangle - \cos\theta|1\rangle\}$, where θ and ϕ both vary from 0 to 2π. For given θ and ϕ, thus a given measurement $\{\Pi_i\}$, we can obtain a matrix $\rho_{A|i} = \frac{\mathrm{Tr}_B(\Pi_i\rho_{AB}\Pi_i)}{\mathrm{Tr}_{AB}(\Pi_i\rho_{AB}\Pi_i)}$ with the probability $p_i = \mathrm{Tr}_{AB}(\Pi_i\rho_{AB}\Pi_i)$ corresponding to the measurement's outcome i. With fixed p_i and $\rho_{A|i}$, we can calculate $\sum_i p_i S(\rho_{A|i})$. The aim in computing the classical correlation is to find the minimum $\sum_i p_i S(\rho_{A|i})$ depending on θ and ϕ. We do it numerically

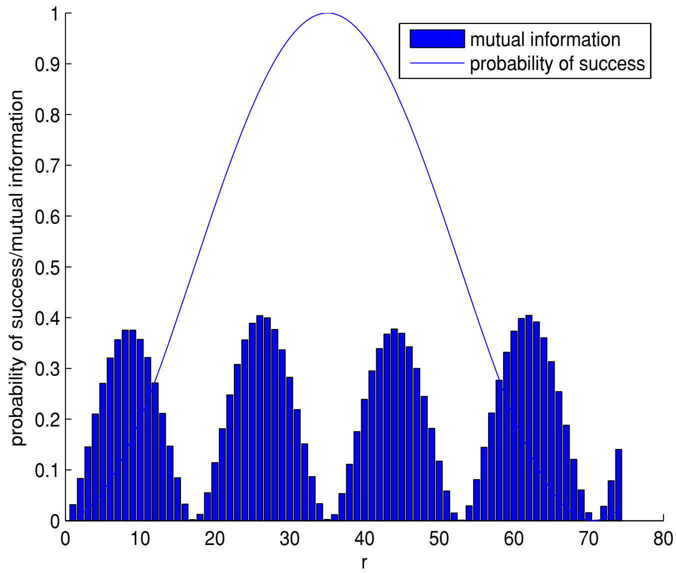

Figure 3. Mutual information between any two qubits for $N = 2048$. The result is obtained numerically using the formula in equation (9) based on the reduced density matrix in equation (14).

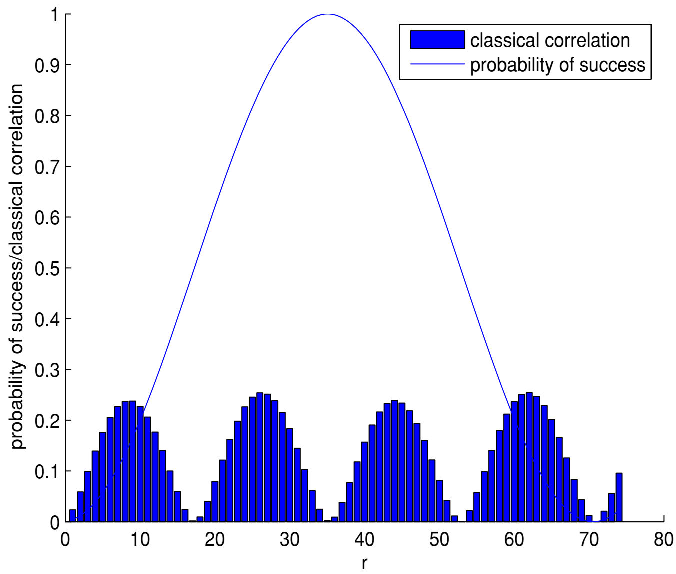

Figure 4. Classical correlation between any two qubits for $N = 2048$. The result is obtained numerically from equation (10). For each density operator, we have done the minimizing procedure to obtain the classical correlation.

by choosing 256 values from 0 to 2π for θ and ϕ respectively. For a density operator ρ_2, we can find its classical correlation by optimizing the measurement (finding optimal θ and ϕ ranging from 0 to 2π). The density operator ρ_2 varies in the Grover search algorithm;

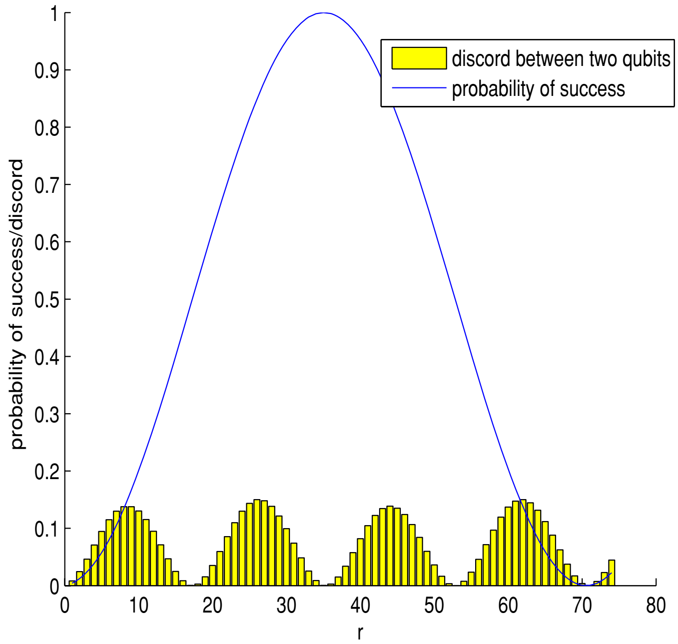

Figure 5. Quantum discord between any two qubits for $N = 2048$. It is the difference between the mutual information and classical correlation.

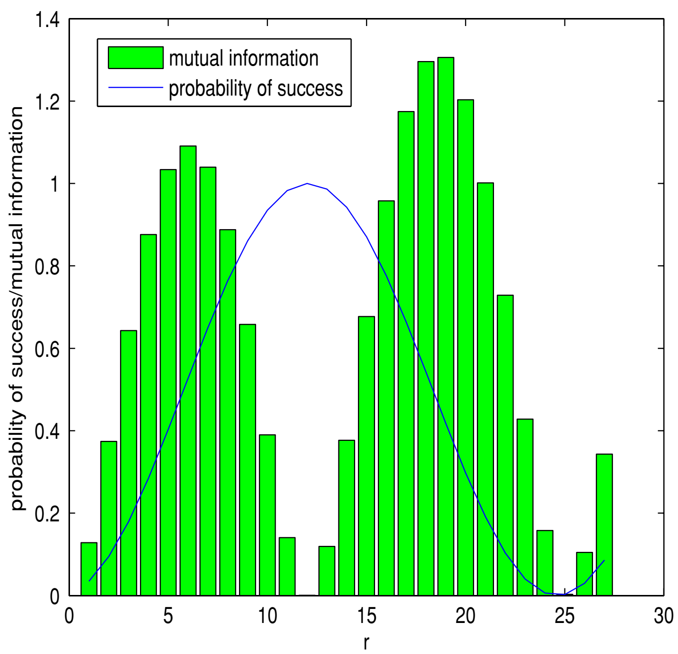

Figure 6. Mutual information between any one qubit and the other seven qubits. We divide the whole n qubits into two parts: the $n - 1$ qubits part A and the one qubit part B, and use the formula in equation (9) to get the numerical result. Here n takes 8.

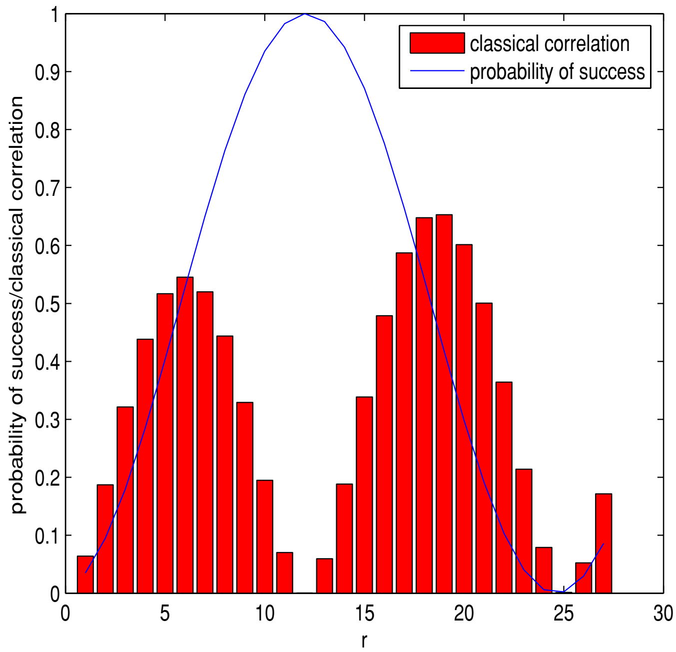

Figure 7. Classical correlation between any one qubit and the other seven qubits. We note that the behavior of the classical correlation and the quantum discord is the same.

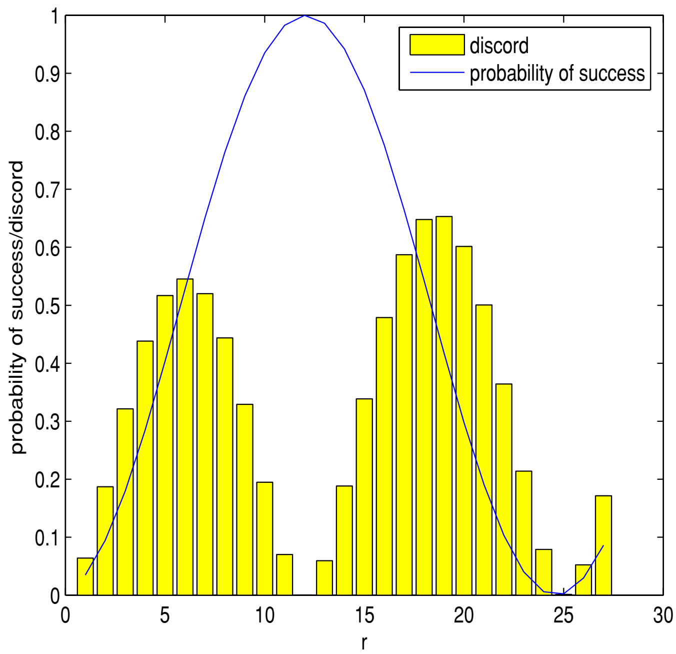

Figure 8. Quantum discord between any one qubit and the other seven qubits.

the evolution of its classical correlation can thus be calculated numerically. The results are presented in figure 4.

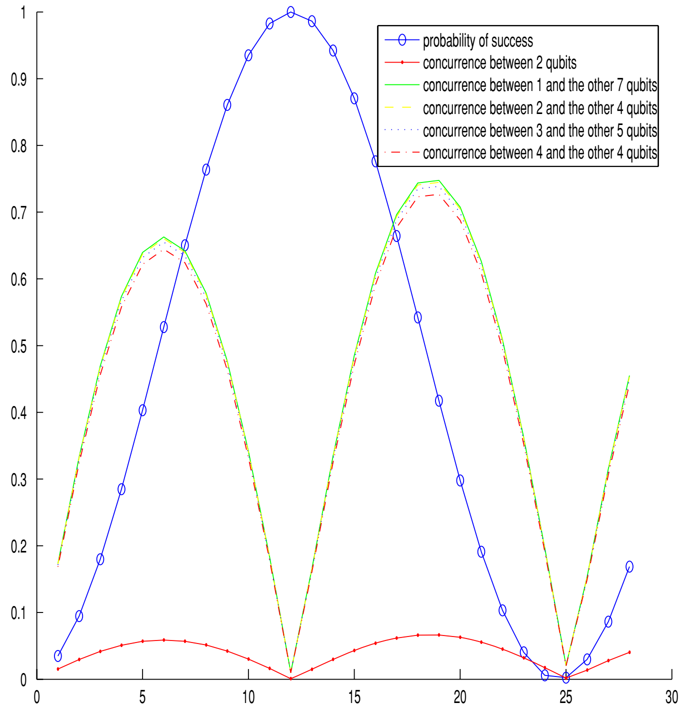

Figure 9. Concurrence between any k and $n-k$ qubits, where $n = 8$ and k varies from 1 to 4. It is seen from the graph that when k varies the curve of concurrence does not change a lot, which suggests that the entanglement between any two parts is not sensitive to how you divide the whole register.

We can find that quantum discord is the difference between the mutual information I and the classical correlation C, see equation (11). The quantum discord can thus be obtained. The numerical results are shown in figure 5, where in all the above we take $N = 2048$.

For the multipartite system, besides the pairwise correlations between any two qubits, other correlations are also of interest. In particular, the pairwise entanglement sharing and other pairwise correlations are monogamy [21, 25–29]; when n tends to infinity all of the pairwise correlations should vanish. Therefore, it should be interesting to view those correlations from a different point. We will next study those correlations between any one qubit and the other $n-1$ qubits. In this situation, we divide the whole n qubits into two parts: the $n-1$ qubits part A and the one qubit part B, where we choose B as the part to be measured when computing the classical correlation and quantum discord.

The calculation is similar to the pairwise case. We first get the $n-1$ qubits reduced density matrix ρ_A and the one-qubit reduced density matrix ρ_B from the whole density matrix ρ_n in equation (13). Then we can calculate the mutual information using equation (9). Since part B is one qubit, we can employ the parameterized measurement bases $\{\cos(\theta)|0\rangle + \mathrm{e}^{\mathrm{i}\phi}\sin\theta|1\rangle, \mathrm{e}^{-\mathrm{i}\phi}\sin\theta|0\rangle - \cos\theta|1\rangle\}$, following the same approach of minimizing the entropy after the measurement on B, the classical correlation and quantum discord can be found numerically. The results are shown in figures 6–8, where we set $n = 8$.

For entanglement, we can also calculate the concurrence between any k and $n-k$ qubits. As can be seen from equation (4) that during the whole process of the Grover search the n-qubit

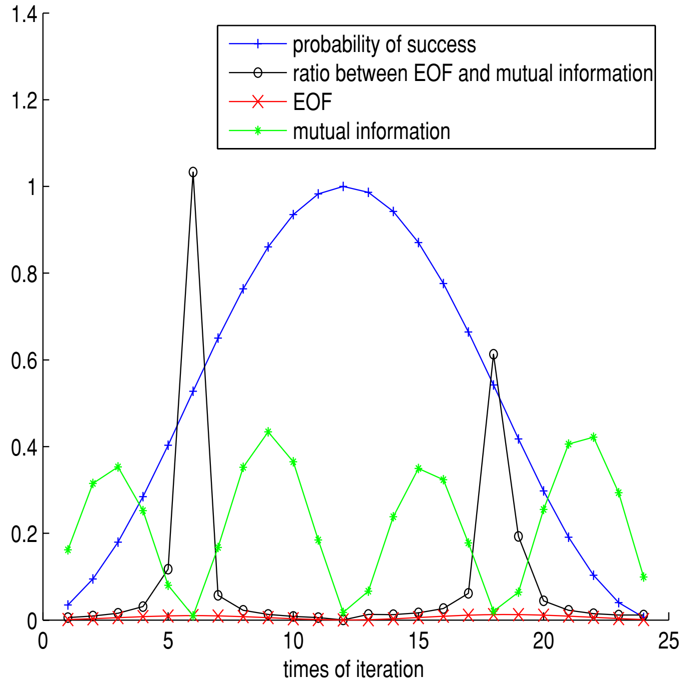

Figure 10. Comparison between EOF and mutual information between any two qubits. $n = 8$.

register state is always a pure state. So we can use equation (8) to calculate the concurrence between any k qubits and the other $n-k$ qubits:

$$C_{k,n-k} = \left(\frac{2^k}{2^k-1}\left[1-\left(a^2+\left(\frac{N}{2^k}-1\right)b^2\right)^2 - 2(2^k-1)\left(ab+\left(\frac{N}{2^k}-1\right)b^2\right)^2 - (1-2^{-k})^2N^2b^4\right]\right)^{1/2}. \tag{16}$$

For explicit, we show these results in figure 9.

It is also of interest to compare entanglement and the mutual information of any two qubits in the whole process. Here we use entanglement of formation (EOF) as the entanglement measurement in place of concurrence, since both mutual information and EOF are defined by means of entropy. We find when EOF gets its maximal mutual information is minimal. The result is shown in figure 10.

4.3. The increasing rate of success probability versus entanglement

The increasing rate is

$$\frac{\partial P}{\partial r} = \alpha\sin((2r+1)\alpha). \tag{17}$$

We find that the increasing rate has an interesting connection with the concurrence between any two qubits in equation (15). Both of them firstly increase with the iteration progress until they get their summit, respectively and then begin to fall. Suppose they get their peak point at

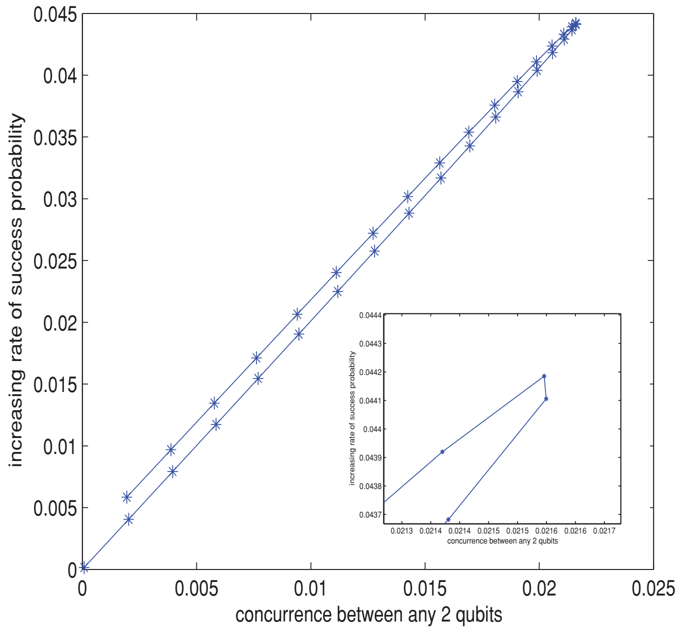

Figure 11. The increasing rate of success probability versus concurrence between any two qubits. Here we take $n = 11$. The part in the vicinity of the peak point is enlarged at the corner.

$r1$, $r2$, respectively. We find that $r1$, $r2$ are connected. From equation (17) we can calculate $r1$ directly. Let $(2r + 1)\alpha = \pi/2$ and remember that r is an integer, so that

$$r1 = CI\left(\frac{1}{2}\left(\frac{\pi}{2\alpha} - 1\right)\right). \tag{18}$$

To calculate $r2$ let $\frac{\partial C_{1,1}}{\partial r} = 0$. We can get

$$r2 = CI\left(\frac{1}{2}\left(\frac{\pi}{2\alpha} - 1.5\right)\right). \tag{19}$$

It can be seen directly from equations (18) and (19) that $r1 - r2 = 0, 1$. We checked that both cases exist, e.g. when the total qubit number $n = 9, 11, 25, 26, 28, 30, \ldots, r1 - r2 = 1$, while n takes other values $r1 - r2 = 0$. The relation between the increasing rate and entanglement is shown in figure 11.

5. Analysis of the results and conclusions

(a) We find that all these correlations mentioned above tend to zero near the point where the success probability of the search runs to 1. This result indicates that when we fulfill the task of searching, we have totally separated the target state. This can easily be understood since when the search succeeds, what we get is the final state (target state) which is a separable pure state. Thus, there are no correlations, quantum or classical. Since the target state is separable, if there are any correlations existing, it means that the target state is not yet obtained. Thus, all correlations being almost zero is necessary for the final step in the search algorithm. (b) We may also note that in the initial state, all correlations are also zero. A naive guess may be that since the target state and a database encoded in other $N - 1$ ($N = 2^n$) states are superposed together in the initial state, the entanglement and the correlations should be in a maximum point. Actually, since the probable states are superposed together with same amplitude, the initial state we prepared takes the form $|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N} |x\rangle$. This is also a separable state. For example, consider state $|\psi\rangle = \frac{1}{\sqrt{d_1 d_2 \ldots d_n}} \sum_{i_1 i_2 \ldots i_n} |i_1 i_2 \ldots i_n\rangle = \left(\frac{1}{\sqrt{d_1}} \sum_{i_1} |i_1\rangle\right) \ldots \left(\frac{1}{\sqrt{d_n}} \sum_{i_n} |i_n\rangle\right)$, this is apparently a separable pure state. Thus, all correlations in the beginning of search are zero. (c) In the process of the search, we may find that the amplitude of the target state becomes large monotonically, while the amplitudes of other states are depressed. Thus, the probability to find the target state is enhanced in the process of the search until it reaches the optimal point, and the probability to find other states are negligible at that time. (d) The entanglement between any two qubits quantified by concurrence firstly increases from zero to a maximal point, then will decrease to zero, see figure 2. On the other hand, the behaviors of classical correlation, quantum discord and the mutual information between two qubits are different from the behavior of the concurrence. After increasing and decreasing for the first time, they repeat the routine for a second time, see figures 3–5. When the concurrence reaches the maximal point, those correlations become zero. Our explanation is that at this case, the correlations in the state are mainly entanglement, quantum discord which also quantifies one property of the quantum correlations does not exist at this point. This fact confirms the original claim in [11] that quantum discord is a complementary quantity to entanglement. (e) When investigating the total system whose state is pure, the behaviors of all correlations between one and the other we find that $n - 1$ qubits are actually the same. This suggests that the pure state correlations can be described by any of the correlation measures. There is no qualitative difference between those measures. (f) When the probability to find the target state is optimal, and all correlations are almost zero, at this time, if we continue the search algorithm, all correlations will increase as presented in our figures. And finally, the state is expected to go back to the initial state. (g) Entanglement is probably the reason for the increase of success probability in the Grover search, i.e. the increasing rate of success probability increases in accordance with entanglement, and it gets its maximum at the same time or immediately after the entanglement approaches its summit. This result is another example and further explanation of the argument by Shimoni, Shapira and Biham in [30, 31], where they applied the Groverian entanglement measure to characterize pure quantum state and argue that the entanglement is found to be correlated with the speedup achieved by the quantum algorithm compared to classical algorithms. This also explains why the power of the Grover search algorithm depends on the ability to generate entanglement in the early stages of its operation and on the ability to remove it when the target state is approached [31].

6. Summary

In this work we have studied several correlations in the whole process of the Grover search and made a comparison among them. The evolution results in the search algorithm obtained are quantities: (i) the concurrence, entanglement of formation, quantum discord, classical correlations and mutual information between any two qubits; (ii) the concurrence between any k qubits and the other $n-k$ qubits; (iii) the quantum discord, classical correlation and mutual information between any one qubit and the other $n - 1$ qubits. We have characterized the Grover search algorithm and showed the results in figures. In particular, in these figures, we gave the evolution of quantum discord in the whole process of the Grover search which to our knowledge had never been obtained before. We also argue that entanglement measured by concurrence works as the indicator of the increasing rate of the success probability.

The role of different kinds of correlations in quantum information processing tasks is an interesting question. We systematically studied evolution of several correlations in the Grover search. It will also be interesting to study correlations in other quantum algorithms.

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