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RAPID COMMUNICATION

Effects of initial states on the quantum correlations in the generalized Grover search algorithm*

Zhen-Yu Chen(陈祯羽)[1], Tian-Hui Qiu(邱田会)[1], Wen-Bin Zhang(张文彬)[2], and Hong-Yang Ma(马鸿洋)[1,†]

[1] *School of Science, Qingdao University of Technology, Qingdao* 266033, *China*

[2] *School of Information and Control Engineering, Qingdao University of Technology, Qingdao* 266033, *China*

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We investigate the correlations between two qubits in the Grover search algorithm with arbitrary initial states by numerical simulation. Using a set of suitable bases, we construct the reduced density matrix and give the numerical expression of correlations relating to the iterations. For different initial states, we obtain the concurrence and quantum discord compared with the success probability in the algorithm. The results show that the initial states affect the correlations and the limit point of the correlations in the searching process. However, the initial states do not influence the whole cyclical trend.

Keywords: Grover search algorithm, quantum correlations, initial states, the success probability

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1. Introduction

Over the past two decades, it was demonstrated that quantum algorithms could solve some non-deterministic polynomial complete problems in polynomial time. Shor's factorization algorithm[1] and Grover's search algorithm[2] show this advantage. And many works have focused on the reason for the quantum speedup.[3,4] Since then, quantum algorithms have been at the forefront of research. There have been many versions of the search algorithm, for instance, the algorithm searching for unknown number of targets,[5] the algorithm used for query-based eigensolver[6] and for image retrieval.[7] However, it quickly became clear that it was not enough to concentrate on quantum algorithms alone, but rather to put a lot of efforts into studying reasons behind their superiority. One widely accepted theory was that quantum entanglement is of particular significance in the algorithms. At that time, entanglement was thought as exactly nonclassical correlations.[8] The statement had been questioned until it was proved that entanglement cannot explain all nonclassical correlations. The separated states also have correlations called quantum discord in the DQCI model.[9–11] Subsequently, correlations as an important source are important to quantum communication and so on.[12–15] And quantum coherence related to correlations is also regarded as a fundamental resource in quantum information processing.[16–19]

Recently, there are many works offering a set of elaborates that quantum entanglement is the key to reducing the time complexity from $O(N)$ to $O(\sqrt{N})$ in the Grover search algorithm.[20] To evaluate the effects on correlations in the algorithm, it would be useful to quantify them in actual application. They are applied to develop measures for bipartite systems, such as concurrence.[21–23] So far, a lot of reports on estimating quantitatively correlations in the algorithm have been published. Most measurements are concerning on bipartite entanglement and multipartite entanglement.[24–28] In terms of concurrence and quantum discord, the correlations in states produced by Grover's iterations were calculated by numerical methods. It was revealed that the excellence of the algorithm is the ability to generate highly-entanglement states in the process and single state when we make measurement.[29] As for global correlations, Batle *et al.* pointed that no quantum correlation boosts the search. Furthermore, the process that first increases and then decreases is a common trend for correlations.[30–32]

The above results show that entanglement plays more significant role in the algorithm than correlations different from it.[33–37] But there are a few studies focused on the comparison about entanglement and correlations in the algorithm with the arbitrary initial states. The algorithm with an arbitrary initial state is one generalization of the origin, considered to study how the initial states influence the correlations. In this paper, we use an entanglement measure concurrence $C(\rho)$ and quantum discord $D(A,B)$ in terms of classical correlation $C(A,B)$ and mutual information $I(A,B)$ to quantity correlations in states produced by iterations.[38,39] In the calculations, to obtain the reduced density matrix is difficult. We could construct a set of suitable bases. Based on the above method, the numerical procedure is applied to numerically cal-

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†Corresponding author. E-mail: hongyang_ma@aliyun.com

culate $\mathcal{C}(\rho)$ and $D(A,B)$ for different initial states. It is found that the curves of correlations repeat twice the process where increases up to approximately half of the optimal number of iterations and then decreases. And it is verified with the uniformed initial states in Ref. [30]. That is, the initial states have little effect on the trend of the correlations.

The paper is organized as follows. In Section 2, the quantum search algorithm with arbitrary initial states is described. In Section 3, the different correlation measures are presented and the calculation procedure of correlations is introduced. In Section 4, the procedure is used to perform calculations for different initial states. In Section 5, the results are summarized.

2. Grover search algorithm with an arbitrary initial state

In the Grover search algorithm, we may adopt an n-qubit quantum register to figure all elements , where $N = 2^n$. Each contains the indices $i = 0, 1, \ldots, n-1$. It is further assumed that the labeled states are exactly solutions to the search problem. Determining whether an element is the labeled state can be represented by the Boolean function $f(i)$. It satisfies $f(i) = 1$ if $|i\rangle$ is the solution, while $f = 0$ for the other states.

First, we introduce an n-qubit register $|i\rangle = |i_0, i_1, \ldots, i_{N-1}\rangle$ and an auxiliary qubit $|q\rangle$ in the computation. A quantum oracle O operates as a black box competent to recognize the labeled elements. The auxiliary qubit flips from $|0\rangle$ to $|1\rangle$ when $|i\rangle$ is a solution or unchanged. It works as follows on computational bases $|i\rangle$ when the ancilla $|q\rangle$ is initially set to the state $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$:

$$O|i\rangle|-\rangle_q = (-1)^{f(i)}|i\rangle|-\rangle_q. \tag{1}$$

Obviously, the labeled states are applied a phase of $-\pi$. Since the auxiliary state does not change, we describe it as $O|i\rangle = (-1)^{f(i)}|i\rangle$ for convenience. We describe the search algorithm in the following.

Step 1 The initialization phase. Prepare the n-qubit register $|0\rangle^{\otimes n}$ and the ancilla $|1\rangle_q$. Then, perform the H gate on each qubit in the n-qubit register and the ancilla

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

The resulting state regarded as the initial state is $|\phi(0)\rangle = \frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}|i\rangle$. The auxiliary qubit is $|-\rangle_q$. Here we discuss an arbitrary, possibly entangled state as the initial state

$$|\varphi(0)\rangle = \sum_{i=0}^{N-1} a_i(0)|i\rangle. \tag{2}$$

Step 2 Grover's iterations. First, the oracle operator is applied, which contributes to the labeled states' phase negative. Because it has no effect on the auxiliary state, the effect can be expressed as

$$I_f^{\pi}|\varphi(0)\rangle = \sum_{i=0}^{N-1}(-1)^{f(i)}a_i(0)|i\rangle. \tag{3}$$

Second, the following three steps are performed: apply the H gate to each qubit in the n-qubit register; rotate the state $|00\cdots0\rangle$ by a phase of π radians; apply the H gate again. They cause all states rotated by π radians around their average amplitude, which is generally described as

$$-H^{\otimes n}I_0^{\pi}H^{\otimes n}|\varphi(0)\rangle = \sum_{i=0}^{N-1}(2\bar{a}(0) - a_i(0))|i\rangle, \tag{4}$$

where $\otimes$ denotes the tensor product, representing to apply the H gate to n qubits, and $\bar{a}(0)$ is the average of the all amplitudes. The operation combining the above two rotations in one Grover iteration is expressed as

$$U_G = -H^{\otimes n}I_0^{\pi}H^{\otimes n}I_f^{\pi}. \tag{5}$$

Step 3 Measurement. Measure the n-qubit register in the computational bases after τ Grover iterations, where τ is the optimal number of iterations in the form

$$\tau = \left\lfloor \left(\frac{\pi}{2} - \sqrt{\frac{r}{N-r}}\right) \Big/ \cos^{-1}(1-2r/N) \right\rfloor, \tag{6}$$

$\lfloor x \rfloor$ does x to round up and round down numbers. The success probability can be expressed as

$$P = N|\bar{a}(0)|^2 + O\left(\frac{1}{\sqrt{N}}\right).$$

The origin Grover search algorithm is usually approximate, and it is only exact when finding one out of four. The phase matching condition could be used to obtain the exact solutions with a restricted arbitrary initial state.[40–42] In general, $P(r)$ is reduced in the algorithm with an arbitrary initial state $|\varphi(0)\rangle$. For the specified solution space, the weighted averages of the amplitudes satisfy the recursion equations.[43] Under these circumstances, the optimal number of iterations is confirmed to be the same as the case where the initial state is $|\phi(0)\rangle$. Whereas, the success probability $P(r)$ is decreased, and, more importantly, it reaches the minimum after τ iterations with some certain initial states.

3. Quantum correlations

3.1. Concurrence

For arbitrary mixed state, concurrence is a well-accepted measure of bipartite entanglement.[44–46] To measure the entanglement in the n-qubit linear register, a convenient method is tracing out $n-2$ qubits and subsequently detecting the concurrence.

Given bipartite density matrix ρ, a new related matrix is obtained by $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^{\dagger}(\sigma_y \otimes \sigma_y)$, where σ_y is the Pauli

matrix which is effective in a phase and bit flip and $\rho^{\dagger}$ indicates the conjugation of ρ. Then concurrence is obtained through the formula

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

All λ_i's are the square roots of the eigenvalues of the matrix $\rho\tilde{\rho}$ and $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$.

3.2. Quantum discord

Quantum discord is the difference between the total correlation and the classical correlation after the measurement. The total correlation is the quantum mutual information expressed in the form[47]

$$I(A,B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \tag{8}$$

Classical correlation between A and B is explained as the maximum information we could obtain from A (B) after measuring B (A).[48] Choose a complete set of projectors $\{\Pi_i\}$ to measure the subsystem A. Correspondingly, the index set $\{i\}$ represents results with the probability of p_i. The state of B after acting the projectors is

$$\rho_{B|i} = \frac{\mathrm{Tr}_A(\Pi_i \rho_{AB} \Pi_i)}{\mathrm{Tr}_{AB}(\Pi_i \rho_{AB} \Pi_i)},$$

and $p_i = \mathrm{Tr}_{AB}(\Pi_i \rho_{AB} \Pi_i)$. For an arbitrary density matrix AB, the choice of measurement proves a decisive factor of the above presentation. That is, the different measurement bases we applied, the different results we obtained. So the biggest amount of information based on the measurement is

$$\begin{aligned} C(A,B) &= \max_{\{\Pi_i\}} \left\{ S(\rho_B) - \sum_i p_i S(\rho_{B|i}) \right\} \\ &= S(\rho_B) - \min_{\{\Pi_i\}} \left\{ \sum_i p_i S(\rho_{B|i}) \right\}. \end{aligned} \tag{9}$$

Thus, quantum discord is mathematically described by

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

3.3. Calculation procedure of quantum correlations

Consider an arbitrary initial state of the real amplitude $|\varphi(0)\rangle$ in the Grover search algorithm. In general, we use $U_0|0\rangle$ to represent the initial state, where U_0 is the unitary transformation. In the origin Grover algorithm, $U_0 = H^{\otimes n}$. When we suppose that $|\varphi(0)\rangle = \sum_{i=0}^{N-1} a_i(0)|i\rangle$, we obtain

$$\begin{aligned} |\varphi(0)\rangle &= \sum_k |i_k\rangle\langle i_k|U_0|0\rangle + \sum_{j\neq i_k} |j\rangle\langle j|U_0|0\rangle \\ &= \sin\beta |A(0)\rangle + \cos\beta |B(0)\rangle, \end{aligned} \tag{11}$$

where $|A(0)\rangle$ is the set of solutions and $|B(0)\rangle$ is the set of the remain states. Easily, we calculate that

$$|A(0)\rangle = \frac{1}{\sin\beta}\left(\sum_k |i_k\rangle\langle i_k|\right) U_0|0\rangle = \frac{1}{\sin\beta}\sum_k U_{0,i_k}|i_k\rangle, \tag{12}$$

$$|B(0)\rangle = \frac{1}{\cos\beta}\left(\sum_{j\neq i_k} |j\rangle\langle j|\right) U_0|0\rangle = \frac{1}{\cos\beta}\sum_{j\neq i_k} U_{0,j}|j\rangle, \tag{13}$$

where $U_{0,i_k} = \langle i_k|U_0|0\rangle$ and $U_{0,j} = \langle j|U_0|0\rangle$. It is considered in this paper that there is only one target state, written as $|i'\rangle$. So we have

$$|A(0)\rangle = \frac{1}{\sin\beta} a_{i'}(0)|i'\rangle, \quad |B(0)\rangle = \frac{1}{\cos\beta}\sum_j a_j(0)|j\rangle,$$

where $\sin\beta = a_{i'}(0), \cos\beta = \sqrt{1-a_{i'}^2(0)}$. And the initial state can be written as $|\varphi(0)\rangle = a_{i'}(0)|A(0)\rangle + \sqrt{1-a_{i'}^2(0)}|B(0)\rangle$. To obtain the density matrix of the total system, it is feasible to select a set of normalized basis of this form

$$|A(r)\rangle = |i'\rangle, \quad |B(r)\rangle = \sum_{j\neq i'} \frac{a_j(r)}{\sqrt{1-a_{i'}^2(r)}}|j\rangle. \tag{14}$$

Based on the above bases, the density matrix is

$$\begin{aligned} \rho &= a_{i'}^2(r)|A(r)\rangle\langle A(r)| + (1-a_{i'}^2(r))|B(r)\rangle\langle B(r)| \\ &\quad + a_{i'}(r)\sqrt{1-a_{i'}^2(r)}(|A(r)\rangle\langle B(r)| + |B(r)\rangle\langle A(r)|) \\ &= (1-a_{i'}^2(r)) \sum_{j_1,j_2\neq i'} \frac{a_{j_1}(r)a_{j_2}(r)}{1-a_{i'}^2(r)}|j_1\rangle\langle j_2| + a_{i'}^2(r)|i'\rangle\langle i'| \\ &\quad + a_{i'}(r)\sqrt{1-a_{i'}^2(r)}\left(\sum_{j\neq i'} \frac{a_j(r)}{\sqrt{1-a_{i'}^2(r)}}(|j\rangle\langle i'| + |i'\rangle\langle j|)\right). \end{aligned} \tag{15}$$

We can get the from of two-qubit reduced density matrix using the above n-qubit one by tracing out any $n-2$ qubits. A widely-used method is to divide the above N-dimensional matrix into four-dimensional matrix with the amount of $2^{n-2} \times 2^{n-2}$ and sum the diagonal elements up. It takes the following form named as $\rho(r)$:

$$\begin{pmatrix} \sum_i a_i^2(r) & \sum_i a_i(r)a_{i+1}(r) & \sum_i a_i(r)a_{i+2}(r) & \sum_i a_i(r)a_{i+3}(r) \\ \sum_i a_i(r)a_{i+1}(r) & \sum_i a_{i+1}^2(r) & \sum_i a_{i+1}(r)a_{i+2}(r) & \sum_i a_{i+1}(r)a_{i+3}(r) \\ \sum_i a_i(r)a_{i+2}(r) & \sum_i a_{i+1}(r)a_{i+2}(r) & \sum_i a_{i+2}^2(r) & \sum_i a_{i+2}(r)a_{i+3}(r) \\ \sum_i a_i(r)a_{i+3}(r) & \sum_i a_{i+1}(r)a_{i+3}(r) & \sum_i a_{i+2}(r)a_{i+3}(r) & \sum_i a_{i+3}^2(r) \end{pmatrix},$$

where $i = \{0,4,\ldots,2^{n-1}\}$. According to the above reduced density matrix, concurrence could be calculated.

Next, we will calculate quantum discord by the definition. The major task is to find the minimum amount of information obtained by one subsystem after measuring the other system. The operator bases could be adopted with the form of $\left\{\cos\theta|0\rangle + e^{i\omega}\sin\theta|1\rangle, e^{-i\omega}\sin\theta|0\rangle - \cos\theta|1\rangle\right\}$, where $0 \le \theta \le 2\pi$ and $0 \le \omega \le 2\pi$. How to find the minimum of this binary function is a crucial step. Apparently, the alignment cannot be obtained in the case in which the amplitudes of states are unknown. Instead, the minimum can be obtained by the steepest descent method with different initial points.

4. Analytical calculations of quantum correlations

4.1. Two-qubit states

Consider a two-qubit state with the real amplitudes in the form

$$|\varphi(0)\rangle = \sum_{i=0}^{3} a_i(0)|i\rangle. \tag{16}$$

We obtain Table 1 about the amplitudes under different iterations, where $\alpha = \sum_{j\neq i'} a_j(0)$. It shows that the success probability to search is periodic, which makes concurrence and quantum discord periodic. Since the elements of the density matrix are invariable whether the amplitudes are positive or negative. Obviously,

$$(\alpha + a_{i'}(0))^2 \ge (\alpha - a_{i'}(0))^2$$

is true when $a_{i'}(0)$ is positive. In this sense, the max probability to search $|i'\rangle$ is expressed as

$$P_{\max} = \max\left\{a_{i'}^2(0), \left(\frac{1}{2}(\alpha + a_{i'}(0))\right)^2\right\}. \tag{17}$$

The best number of iteration is one in Eq. (6), while it is true only when $(\frac{1}{2}(\alpha + a_{i'}(0)))^2 \ge a_{i'}(0)^2$. Discussing the case where the initial state is $|i'\rangle$ is meaningless. To make $P_{\max} = 1$, the amplitudes satisfy the condition $\alpha + a_{i'}(0) = 2$ that the superposition state of a uniform amplitude distribution $|\phi(0)\rangle$ meets. And the algorithm works best in the circumstances resulting in concurrence and quantum discord almost equal to zero when $r = 1$.

Based on the reduced density matrix, concurrence has the following analytic equation:

$$\mathcal{C}(\rho) = 2\left|a_0(r)a_3(r) - a_1(r)a_2(r)\right|. \tag{18}$$

In terms of quantum discord, the two-qubit reduced matrix ρ_{AB} has eigenvalues $\{0,0,0,1\}$, while the one-qubit reduced matrix $\rho_{A(B)}$ has eigenvalues $\frac{1}{2}(1 \pm \sqrt{1-\mathcal{C}(\rho)^2})$. Finding θ and ω to realize the minimum relies on computers for help. Obviously, the eigenvalues of $\rho_{A(B)}$ are $\{0,1\}$ when $\mathcal{C}(\rho) = 0$.

Table 1. The amplitudes in all states when $N = 4$.

r	0	1	2	3
$a_{i'}(r)$	$a_{i'}(0)$	$\frac{1}{2}(\alpha + a_{i'}(0))$	$\frac{1}{2}(\alpha - a_{i'}(0))$	$-a_{i'}(0)$
$a_j(r)$	$a_j(0)$	$\frac{1}{2}(\alpha - a_{i'}(0)) - a_j(0)$	$\frac{1}{2}(-\alpha - a_{i'}(0)) + a_j(0)$	$-a_j(0)$

4.2. Multiple-qubit states

4.2.1. The same amplitude of k unlabeled states

The states with the same amplitude of k unlabeled states take the form

$$|\varphi(0)\rangle = \frac{1}{2}|i'\rangle + \frac{\sqrt{3}}{2\sqrt{k}}\sum_{i=0,i\neq i'}^{k}|i\rangle. \tag{19}$$

These states are useful to study the evolution of the correlations, which have the same amplitude of unlabeled states but the changed sum to the amplitudes in all unlabeled states. In Figs. 1–5 we present the correlations of the states $|\varphi(r)\rangle$, generated by $r = 0,1,\ldots,10$ iterations with the given form of the initial states when $N = 16$. We have the following results.

First, we find $\tau = 1$ when $0 < k < 5$, while when $4 < k < 16$, $\tau = 2$. However, the above results are inconsistent with the results that is $\tau = 3$ when $N = 16$ calculated by Eq. (6). When the initial state is $|\phi(0)\rangle$, one U_G has effects on rotating $|\phi(0)\rangle$ by γ to the target state $|i'\rangle$, where $\gamma = 2\arccos\sqrt{(1-\frac{1}{N})}$. The best number of iterations is defined by the statement that $\tau\gamma + \frac{\gamma}{2} \approx \frac{\pi}{2}$. While when we take $|\varphi(0)\rangle$ as the initial state, it is rotated by π around the average of the initial amplitudes in Eq. (4). Equation (6) does not work in the circumstances. In Ref. [36], the equality relationship $a_{i'}(r+1) = \frac{2}{N}(\sum_{j\neq i'} a_j(r) - a_{i'}(r)) + a_{i'}(r)$ establishes. Obviously, the following condition is true:

$$\left(\sum_{j\neq i'} a_j(r) - a_{i'}(r)\right)a_{i'}(r) \le 0 \Rightarrow P(r+1) \le P(r). \tag{20}$$

And determining if r is an extreme needs to satisfy the following condition:

$$\left(\sum_{j\neq i'} a_j(r-1) - a_{i'}(r-1)\right)\left(\sum_{j\neq i'} a_j(r) - a_{i'}(r)\right) > 0. \tag{21}$$

Second, there is an almost same period since $P(6)$ closes to $(a_{i'}(0))^2$, but is not equal. In the above subsection, $a_{i'}(0) = -a_{i'}(3)$ when $N = 4$. The amplitudes before $r = 7$ are given in Table 2. We can verify that the success probability is no strict periodicity with the initial states listed when $N = 16$.

Third, we find that correlations reach the maximum when $r = 3$ or $r = 10$. It is possible that larger values will be obtained after more iterations. In Ref. [18], the correlations repeat the process that is firstly increase and then decrease twice, yet the curves of P just repeat once. This pattern becomes apparent when we focus on a complete ascending and descending curve of P.

Table 2. The amplitudes in all states when $N = 16$.

r	0	1	2	3	4	5	6
$a_{i'}(r)$	$\frac{1}{2}$	$\frac{\sqrt{3k}+7}{2^4}$	$\frac{7\sqrt{3k}+17}{2^6}$	$\frac{33\sqrt{3k}+7}{2^8}$	$\frac{119\sqrt{3k}-223}{2^{10}}$	$\frac{302\sqrt{3k}-1673}{2^{12}}$	$\frac{220\sqrt{3k}-8143}{2^{14}}$
$a_{j_0}(r)$	0	$\frac{\sqrt{3k}-1}{2^4}$	$\frac{-\sqrt{3k}-7}{2^6}$	$\frac{9\sqrt{3k}-33}{2^8}$	$\frac{-49\sqrt{3k}-119}{2^{10}}$	$\frac{25\sqrt{3k}-305}{2^{12}}$	$\frac{-1088\sqrt{3k}-231}{2^{14}}$
$a_{j_1}(r)$	$\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(1)-\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(2)+\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(3)-\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(4)+\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(5)-\frac{\sqrt{3}}{2\sqrt{k}}$	$a_{j_0}(6)+\frac{\sqrt{3}}{2\sqrt{k}}$

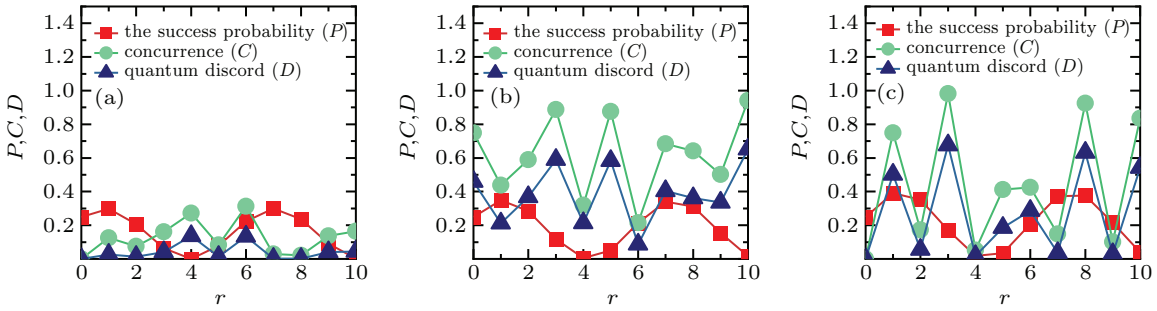

Fig. 1. Concurrence (green line with round points) and quantum discord (blue line with triangular points) compared with the success probability (red line with square points) in the case which the initial states take the form of Eq. (19): (a) $k = 1$, (b) $k = 2$, (c) $k = 3$.

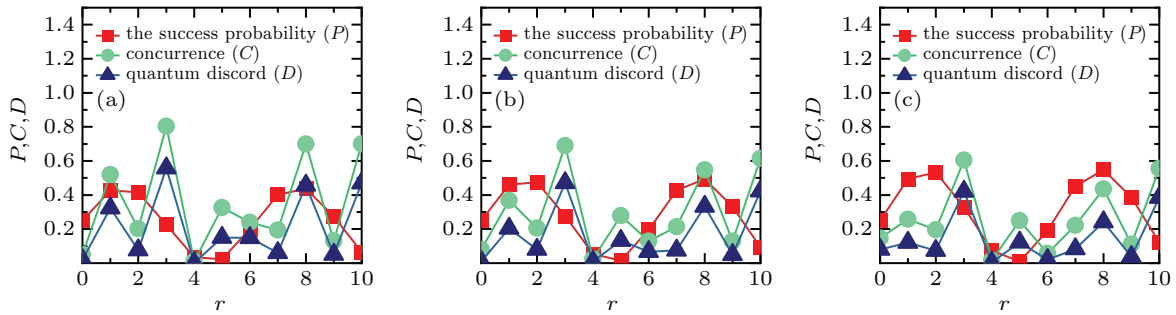

Fig. 2. Concurrence (green line with round points) and quantum discord (blue line with triangular points) compared with the success probability (red line with square points) in the case which the initial states take the form of Eq. (19). (a) $k = 4$; (b) $k = 5$; (c) $k = 6$.

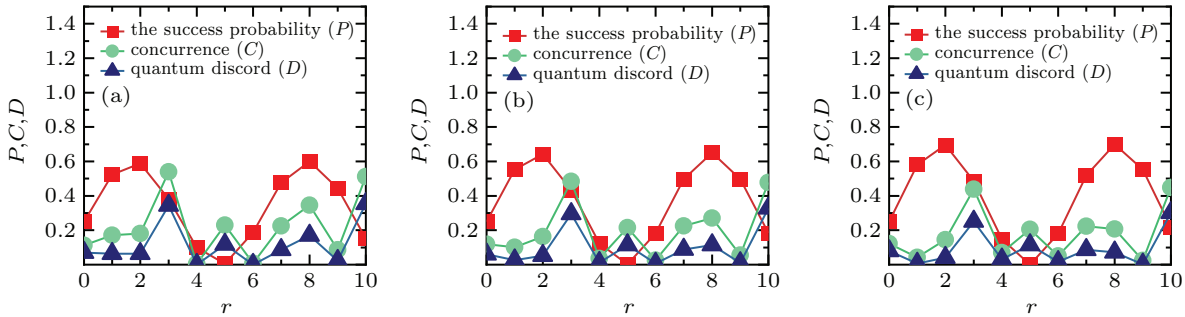

Fig. 3. Concurrence (green line with round points) and quantum discord (blue line with triangular points) compared with the success probability (red line with square points) in the case which the initial states take the form of Eq. (19): (a) $k = 7$, (b) $k = 8$, (c) $k = 9$.

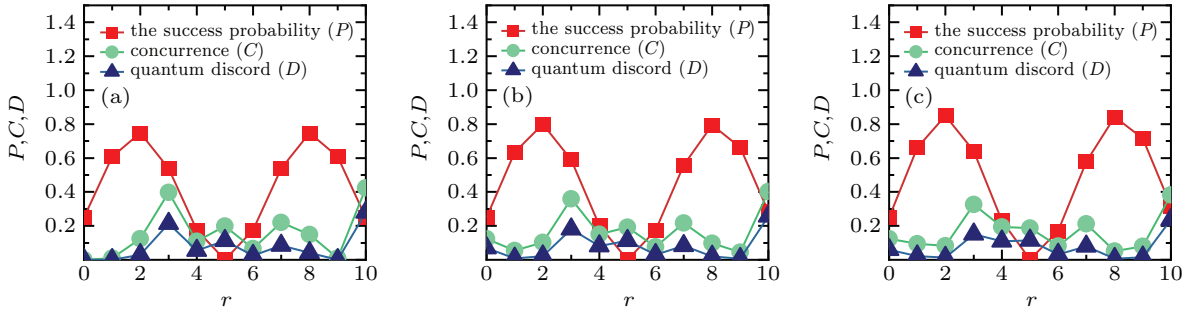

Fig. 4. Concurrence (green line with round points) and quantum discord (blue line with triangular points) compared with the success probability (red line with square points) in the case which the initial states take the form of Eq. (19): (a) $k = 10$, (b) $k = 11$, (c) $k = 12$.

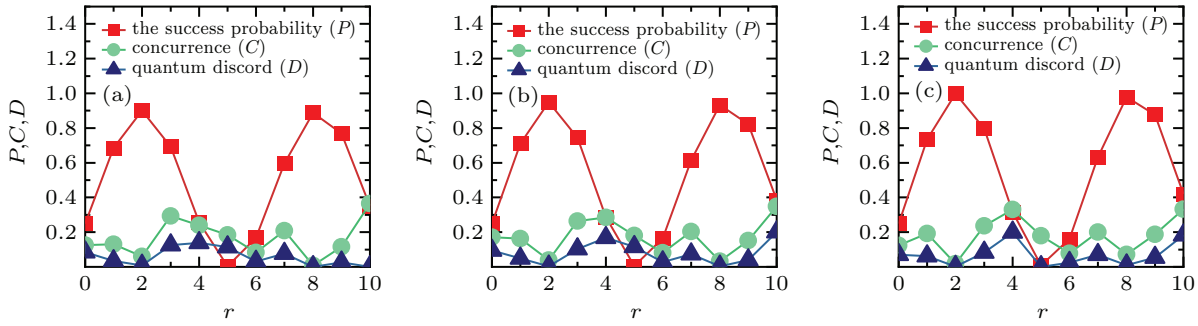

Fig. 5. Concurrence (green line with round points) and quantum discord (blue line with triangular points) compared with the success probability (red line with square points) in the case which the initial states take the form of Eq. (19): (a) $k = 13$, (b) $k = 14$, (c) $k = 15$.

4.2.2. The general n-qubit states

Consider a random pure state with the form of Eq. (3). Since the calculations of concurrence and quantum discord both depend on the reduced density matrix, we analyze the amplitudes consisting of the elements of the matrix when $N \to \infty$. The weighted averages of the two sets satisfy the following recursion equations:

$$\begin{pmatrix} \bar{A}'(r) \\ \bar{B}'(r) \end{pmatrix} = \begin{pmatrix} \frac{N-2}{N} & \frac{2N-2}{N} \\ -\frac{2}{N} & \frac{N-2}{N} \end{pmatrix}^r \begin{pmatrix} \bar{A}'0) \\ \bar{B}'(0) \end{pmatrix}, \tag{22}$$

where the weighted averages are respectively expressed as[42]

$$\bar{A}'(r) = \sqrt{N} a_{i'}(r), \quad \bar{B}'(r) = \frac{\sqrt{N}\sum_{i\neq i'} a_i(r)}{N-1}. \tag{23}$$

It is obvious that in the limit of $N \to \infty$ the matrix could be expressed as

$$\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}^r = \begin{pmatrix} 1 & 2^r \\ 0 & 1 \end{pmatrix}. \tag{24}$$

We use the above matrix in order to obtain the following equation:

$$\bar{A}'(r) = \bar{A}'(0) + 2^r \bar{B}'(0), \quad \bar{B}'(r) = \bar{B}'(0),$$

that indicates the sum up to the amplitudes of the unlabeled states remains nearly unchanged. Just only when $2/N$ is very closed to zero, we can ignore the sign which could make the elements negative. Thus, the success probability increases slowly, since $\tau \to \infty$. If we ideally assume that they are constant, then only the values in terms of the amplitude of the target state in the reduced density matrix will change. Suppose

$$\sigma(r) = \frac{\sum_{i\neq i'} a_i(0)}{N-1} 2^r, \quad \mod(i', 4) = 0,$$

the reduced density matrix takes the form of $\rho(r) = \rho(0) + \widehat{\rho}(r)$, where

$$\widehat{\rho}(r) = \begin{pmatrix} \sigma(r)^2 + 2a_{i'}(0) & \sigma(r)a_{i'+1}(0) & \sigma(r)a_{i'+2}(0) & \sigma(r)a_{i'+3}(0) \\ \sigma(r)a_{i'+1}(0) & 0 & 0 & 0 \\ \sigma(r)a_{i'+2}(0) & 0 & 0 & 0 \\ \sigma(r)a_{i'+3}(0) & 0 & 0 & 0 \end{pmatrix}. \tag{25}$$

Regard $\widehat{\rho}(r)$ as the perturbation term caused by the increasing number of iterations. So we get the matrix $\tilde{\rho}(r) = (\sigma_y \otimes \sigma_y)(\rho(0) + \widehat{\rho}(r))^\dagger(\sigma_y \otimes \sigma_y)$ relevant to concurrence. Because matrix multiplication is distributive, it is obvious that $\tilde{\rho}(r) = (\sigma_y \otimes \sigma_y)\rho(0)^\dagger(\sigma_y \otimes \sigma_y) + (\sigma_y \otimes \sigma_y)\widehat{\rho}^\dagger(\sigma_y \otimes \sigma_y)$. However, we cannot obtain $\lambda_A + \lambda_B = \lambda_{A+B}$ in the case that the eigenvectors of A and B cannot be determined to be equal. The same is true that the equation $\lambda_{\rho(0)} + \lambda_{\widehat{\rho}(r)} \neq \lambda_{\rho(0)+\widehat{\rho}(r)}$ makes the detailed discussion difficult for quantum discord.

However, it is worth noting that each entry in the matrix $\widehat{\rho}(r)$ is related to the function $\sigma(r)$. According to the initial state, the function has the relation of inequality described as

$$0 \leq \sigma(r) \leq \sum_{i\neq i'} a_i(0). \tag{26}$$

That is, the perturbation term is constrained by the initial state, in the sense that $\widehat{\rho}(r)$ has very little effect on the concurrence and quantum discord if $r \ll n$. Under the circumstances, they still remain the cyclical trend. As r gets closer and closer to n, $\sigma(r)$ is growing closer to $\sum_{i\neq i'} a_i(0)$. In that limit, $\widehat{\rho}(r)$ is almost the numerical matrix whose elements are completely determined by the initial states. One situation can be foreseen that the trend of the correlations may still remain periodic, but their values would change.

5. Conclusion

In this paper, we focused on the correlations in the search algorithm with any given initial states $|\varphi(0)\rangle$. Concurrence and quantum discord were applied to characterize pure multiple-qubit states. The suitable bases were developed to perform analytically the reduced density matrix crucial to the correlations. We calculated the correlations of the intermediate states obtained in the evolution of Grover's algorithm using

different initial states. It was found that the initial states affect the correlations and the limit point of the correlations in the searching process. However, the initial states do not influence the whole cyclical trend. In addition, a very important conclusion was that although the arbitrary initial states will reduce the success probability, it will almost reach 100% when the initial state meets certain conditions that we calculate when $N = 4$. In this case, correlations are relatively small compared with $P(r)$. With the general initial states, the evolution of correlations and the conditions to make $P_{\max} = 1$ are also worth exploring.

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