Exact Quantum Search by Parallel Unitary Discrimination Schemes

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Abstract

We study the unsorted database search problem with items $N$ from the viewpoint of unitary discrimination. Instead of considering the famous $O(\sqrt{N})$ Grover’s bounded-error algorithm for the original problem, we seek for the results about the exact algorithms, i.e., the ones succeed with certainty. Under the standard oracle model $\sum_i (-1)^{f(x_i)}|i\rangle|\psi_i\rangle$, we demonstrate a tight lower bound $\frac{2}{\delta} N + o(N)$ of the number of queries for any parallel scheme with unentangled input states. With the assistance of entanglement, we obtain a general lower bound $\frac{2}{\delta} (N - \sqrt{N})$. We provide concrete examples to illustrate our results. In particular, we show that the case of $N=6$ can be solved exactly with only two queries by using a bipartite entangled input state. Our results indicate that in the standard oracle model the complexity of exact quantum search with one unique solution can be strictly less than that of the calculation of OR function.

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I. INTRODUCTION

Quantum computing is more powerful than classical computing due to many peculiar features of quantum mechanics such as superposition and entanglement. Although its theory is still unclear whether quantum computer can efficiently solve NP-complete problem, there do exist some problems for which quantum algorithms outperform any known classical algorithms. Outstanding instances include the Shor’s algorithm for factoring large integers\textsuperscript{1}, and the Grover’s algorithm for searching a specific element in an unsorted database\textsuperscript{2}.

The Unsorted Database Search Problem can be formulated as follows. Suppose we have a database whose elements are labeled from 1 to $N$, and suppose we have a function $f$: $\{1, \cdots, N\} \rightarrow \{0, 1\}$. Assume there is a unique element $x_0$ in the database such that $f(x_0) = 1$. The goal of the problem is to figure out $x_0$ with the minimum number of calculations of $f$.

Usually, we treat the function $f$ as a black-box or an oracle. We use a query to the oracle to get the value $f(x_i)$ when the input to the oracle is $x_i$. In classical computing, the minimum number of queries to the oracle is used to measure the complexity of the original problem. In quantum computing, we use the counterpart of the classical oracle, namely the quantum oracle. A standard quantum oracle $O_f$ for a boolean function $f$ on $\{1, \cdots, N\}$ is defined as follows:

\[ O_f |x\rangle|y\rangle = |x\rangle|y \oplus f(x)\rangle, \]

where $\{|x\rangle : 1 \leq x \leq N\}$ is an orthonormal basis for the principal quantum system of interest, and $\{|y\rangle : y = 0, 1\}$ is an orthonormal basis for the auxiliary qubit which is used to store the result of query. If we prepare the auxiliary system in state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$, the action of $O_f$ on the principal system can be simplified to the following form:

\[ O_f = \sum_{j=1}^{N} (-1)^{f(j)} |j\rangle\langle j|. \]

A general quantum network with $t$ queries can be visualized in Fig. 1, where $O_f$ stands for the quantum oracle, and each $X_i$ is a known unitary operation inserted between two successive queries of the oracle. The input to the network is $|\psi\rangle$ with $m+n$ qubits where the first $m$ qubits represent the auxiliary qubits, and the last $n$ qubits are the qubits relative to the oracle. $X_i$ will affect on $m+n$ qubits while $O_f$ will only affect the last $n$ qubits. The computation is completed with a measurement on the final output state $|\phi\rangle$.

\[ |\phi\rangle = \sum_{i=0}^{N-1} (-1)^{f(i)} |i\rangle. \]

FIG. 1: Illustration of Quantum Network with $t$ queries.

The computation with oracles has the fixed set of output states $\{|\phi_i\rangle\}$ and the same input state $|\psi\rangle$. Thus, the output state of the computation $|\phi\rangle$ relies only on the quantum oracle $O_f$, namely the function $f$. As introduced in Eq. (1), the function $f$ will determine $O_f$ and thus the output state $|\phi\rangle$, which is named $|\phi_f\rangle$. Different function $f_i$ will result in different output state $|\phi_i\rangle$. For an exact algorithm, we need to distinguish the set of output states $\{|\phi_i\rangle\}$ with certainty. In other words, any two states $|\phi_i\rangle$ and $|\phi_j\rangle$ such that $i \neq j$ should be orthogonal. If this orthogonality condition cannot be satisfied, the algorithm will fail to distinguish

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all the possible output states. In such case, $\langle \phi_j | \phi_i \rangle \neq 0 \ (i \neq j)$, the algorithm may output $i$ if the actual result is $j$ and vice versa with some positive probability. If the probability satisfies certain requirements, we call such algorithm a *bounded-error* algorithm. It should be noted that the number of queries used in this network is the measure of the computational complexity.

Grover [2] invented an efficient algorithm to the unsorted database search problem using the quantum network above. More precisely, in his scheme, $m = 0$, namely no auxiliary qubits. All $X_i$ and $O_f$ will affect on the last $n$ qubits. Using the notations above, we have:

$$| \phi_f \rangle = X_l O_f X_{l-1} O_f \cdots X_1 O_f X_0 | \psi \rangle,$$

(3)

Furthermore, $O_f$ in this problem has the form below:

$$O_f = \sum_{j=1}^{N} (-1)^{x_0 j} |j \rangle \langle j|,$$

(4)

where $\delta_{ab}$ or $\delta_{a}^b$ equals to 1 if $a = b$ and equals to 0 otherwise, and $x_0$ is the unique $x$ such that $f(x) = 1$. With a careful choice of $\{X_i\}$ and input state $|\psi\rangle$, Grover obtained a *bounded-error* algorithm using only $O(\sqrt{N})$ queries. Pioneering work in Ref. [3] presented a lower bound of $\Omega(\sqrt{N})$ [15]. Combined with Zalka’s work [3], it immediately implies the Grover’s algorithm is optimal for bounded-error setting. However, the original Grover’s algorithm succeeds with certainty only when $N = 4$.

For exact algorithm, under the oracle model $\sum_j (-1)^{x_0 j} |j \rangle \langle j|$, people obtained the complexity of the decision version of quantum search problem with multi-solution, where they treated the decision version problem as the calculation of function OR [11]. In such situation, $\Omega(N)$ queries is required to get the answer with certainty. However, in this paper, we care about the quantum search problem with unique-solution. Thus, the complexity is no more than $\Omega(N)$. In classical computing, $N - 1$ is necessary for exact algorithm. As the generalization of Grover’s quantum search algorithm, quantum amplitude amplification was proposed in [3]. Later, arbitrary phase concept was introduced [7, 8, 9] under the modified oracle model $\sum_j e^{ibx_0 j} |j \rangle \langle j|$, where $i = \sqrt{-1}$. Hoyer [9] and Long [4] further employed such concept and successfully found an exact algorithm using $O(\sqrt{N})$ queries to solve the quantum search problem. Also, the computing problem of boolean function OR is thought to have a close relation with the unsorted database search problem [10]. Quantum lower bounds for such boolean functions have been thoroughly discussed in Ref. [11].

Another interesting problem which has received considerable attention is the discrimination of unitary operations. Suppose that we have an unknown unitary operation $U$ which is secretly chosen from a set of pre-specified unitary operations, say, $\{U_1, \cdots, U_N\}$. Our task is to decide the real identity of this unitary, i.e. the index of $U$. To do this, we employ a similar network as Fig. [4] with the change that replacing $O_f$ by $U$. In particular, we call the network a *parallel scheme* if the network is reduced to the form of $U^{\otimes t}$. See Fig. [2].

To verify that a parallel scheme is a special case of quantum network, one only needs to notice the identity

$$U^{\otimes 2} = (I \otimes U) S (I \otimes U) S^\dagger,$$

where $S$ is the swap operation, i.e., $S | \psi \rangle | \phi \rangle = | \phi \rangle | \psi \rangle$ for any $| \psi \rangle$ and $| \phi \rangle$. See Fig. [3] for an intuitive illustration.

When the unknown unitary is $U_k$, we obtain $| \phi_k \rangle$ as the output of the discrimination network. To perfectly distinguish between $\{U_k\}$, we need to distinguish among $\{| \phi_k \rangle \}$. So all these states should be mutually orthogonal. The number of $U$ appearing in this network, or the number of runs of $U$ is the cost of the network. Due to its special structure, a parallel scheme can accomplish the discrimination with a single step when a large number copies of $U$ are available.

Unlike the discrimination of nonorthogonal states, which is impossible even arbitrarily large but finite number of copies are available, we can always discriminate any finite set of unitary operations with certainty using some quantum network. Actually it is possible to achieve a perfect discrimination between unitary operations by a parallel scheme [14, 15] with the assistance of a multipartite entangled state as input. Interestingly, it was further proven that the entangled input state is not necessary by employing a sequential scheme instead of a parallel one [16]. An analytical expression for the minimal number of runs needed for a perfect discrimination between two unitary operations using general quantum network was also obtained in Ref. [16]. Very recently it was shown that any two multipartite unitary operations can always be perfectly distinguished by local operations and classical communication [17].
unitary operations is actually the quantum counterpart of oracle identification problem in classical computing. Many works have been done in order to sharpen our understanding of both classical and quantum oracle identification problem [12, 13].

The purpose of the paper is to study the unsorted database search problem from the viewpoint of unitary operation discrimination. It is easy to see the original problem is equivalent to find which \( f_i \) is currently in use, namely an oracle identification problem, which we name it Grover’s Oracle Identification Problem. We want to solve the problem with oracles in Eq. (3) with certainty using a parallel discrimination scheme. For unsorted database problem, the candidate set is \( \{O_i: 1 \leq i \leq N\} \) where \( O_i \) is in the form of Eq. (4) and \( N \) is the size of the database in the problem.

The known quantum lower bound for the problem in discussion is \( \Omega(N) \). It is somewhat surprising that we can solve the Grover’s oracle identification problem by a parallel discrimination scheme without entanglement using at most \( \frac{4}{7}N + 2 \) queries, which is strikingly different from the classical setting, where \( N - 1 \) queries are necessary. We further show that such a scheme is optimal for any parallel scheme without entanglement. We also find that entanglement may reduce the number of queries and thus improve the efficiency of discrimination. In particular, a lower bound \( \frac{1}{2}(N - \sqrt{N}) \) for the discrimination with entanglement is obtained. Most interestingly, we show that two queries are sufficient for a perfect discrimination for \( N = 5 \) without use of entanglement, and are still sufficient for a perfect discrimination for \( N = 6 \) if an entangled input state is allowed. It is also worth noting that in our proofs we have extensively employed the techniques from the graph theory and combinatorics. We hope these proof techniques may be useful for other problems in quantum computation and quantum information.

II. PARALLEL DISCRIMINATION SCHEME FOR EXACT QUANTUM SEARCH

A parallel discrimination scheme which is visualized in Fig. 4 uses the network \( U^\otimes t \) where \( U \) is the unitary operation to identify from a candidate set and \( t \) is the number of the copies, namely the complexity of the scheme. More precisely, in Grover’s Oracle Identification Problem, the candidate set is \( \{f_i\} \) where \( f_i = \sum_j (-1)^{h_{ij}}|j\rangle \langle j| \), the set of possible output states of the network is \( \{f_i^\otimes t|\psi\rangle\} \). Since the algorithm is exact, these output states should be orthogonal to each other. That is,

**Discrimination Condition**: For any \( 1 \leq i < j \leq N \),

\[
\langle \psi|(f_i^\otimes t)^\dagger(f_j^\otimes t)|\psi\rangle = 0,
\]

where

\[
(f_i^\otimes t)^\dagger(f_j^\otimes t) = \sum_{\vec{a}} (-1)^{\tau(\vec{a})}|\vec{a}\rangle \langle \vec{a}|,
\]

where \( \vec{a} = a_1 \cdots a_t \) and

\[
\tau(\vec{a}) = \sum_{k=1}^{t} (\delta_{a_k}^i + \delta_{a_k}^j) \mod 2.
\]

In the following, we will first show the case with only one-copy state. Using one-copy state as a product state block, we obtain a product state discrimination scheme and prove its optimality. Finally, we deal with the scheme with entanglement and give examples.

A. A key lemma

Suppose \( |\psi\rangle \) is an input state in \( \mathcal{H}_N \). We say that \( |\psi\rangle \) can discriminate a pair \( (i,j) \) if \( f_i|\psi\rangle \) and \( f_j|\psi\rangle \) are orthogonal. Note that here a pair \( (i,j) \) is just an abbreviation for \( \{i,j\} \). Let \( S_{|\psi\rangle} \) represent the pairs that can be discriminated by \( |\psi\rangle \), i.e.,

\[
S_{|\psi\rangle} = \{(i,j) : \langle f_i^\dagger f_j |\psi\rangle = 0\}.
\]

With the above notation, we can visualize the discrimination power of \( |\psi\rangle \) by the discrimination graph defined as follows.

**Discrimination Graph**: an undirected graph \( G_{|\psi\rangle} = (V,E) \) with vertex set \( V = \{1, \cdots , N\} \) and edge set \( E = S_{|\psi\rangle} \). We find that such a graph representation may be helpful in understanding the following arguments.

Assume that \( |\psi\rangle \) is of the form \( \sum_i p_i |i\rangle \), where \( \sum_i |p_i|^2 = 1 \). By Eq. (5), we can easily see that \( |\psi\rangle \) can discriminate a pair \( (i,j) \) if and only if

\[
|p_i|^2 + |p_j|^2 = \frac{1}{2}.
\]

Three kinds of interesting states which satisfy the above condition for certain pairs \( (i,j) \) are as follows:

- \( |\psi\rangle = \frac{1}{\sqrt{3}}(|a\rangle + |b\rangle + |c\rangle + |d\rangle) \) with distinct \( \{a, b, c, d\} \) can discriminate any pair in \( \{a, b, c, d\} \). We denote such states as \( K_4\{a, b, c, d\} \) or \( K_4 \) in short. See Fig. 4.

![Fig. 4: Illustration of \( S_{K_4(1,2,3,4)} \), \( N = 6 \).](image)

- \( |\psi\rangle = \frac{1}{\sqrt{2}}(|i\rangle + |j\rangle) \) with distinct \( i, j \) can discriminate any pair \( (i,k) \) or \( (j,k) \) where \( k \notin \{i, j\} \), however the pair \( (i, j) \) cannot be discriminated. We denote such states as \( <i,j> \). See Fig. 5.

- \( |\psi\rangle = a|i\rangle + b \sum_{j \neq i} |j\rangle \), where \( a = \sqrt{\frac{N-3}{2(N-2)}} \) and \( b = \sqrt{\frac{1}{2(N-2)}} \) for \( N \geq 3 \). This state discriminates
due to Eq. 9, we have |K which can be discriminated. In both cases, pairs in i,k can replace i,j ond case is that there are three pairs (i,j) or (i,k) respectively to replace |ψ⟩. Because for the pair (i,j) or (i,k), the other pairs should also not be disjointed with it, there are only three cases which satisfy the assumption. The first case is that only one pair (i,j) can be discriminated. The second case is that there are three pairs (i,j),(i,k) and (j,k) which can be discriminated. In both cases, K₄{i,j,k,l} can replace |ψ⟩. The third case is that |ψ⟩ discriminates the pairs in \{i,c\},c \neq i or \{(c,j),c \neq j\}, then we can use E(i) or E(j) respectively to replace |ψ⟩.

Case 2. If there are two disjointed pairs (a,b), (c,d), due to Eq. 9 we have \|p_a|^2 + \|p_b|^2 = \frac{1}{2} and \|p_c|^2 + \|p_d|^2 = \frac{1}{2}, namely \|p_a|^2 + \|p_b|^2 + \|p_c|^2 + \|p_d|^2 = 1, which implies other \ p_c = 0. In order to satisfy the condition above, at least one variable in each equation is non-zero. If there are only 2 (say \ p_a, p_c) or 4 variables are non-zero, then we can use < a, c > or K₄ to replace |ψ⟩ respectively. Otherwise, we have p_a, p_b, p_c non-zero, < a, c > is also able to replace |ψ⟩.

In both cases |ψ⟩ can be replaced successfully. That completes the proof.

As a direct consequence of Lemma 1, the power to discriminate all the pairs one-copy state cannot exceed the power of K₄ or < i, j > or E(i). Thus, one-copy state isn’t adequate for discrimination when \( N \geq 5 \). It is easy to verify that there is no discrimination scheme for the cases of \( N = 2, 3 \). Only for \( N = 4 \) we have a discrimination scheme with using one single copy. However, if we choose another oracle model say the auxiliary qubit |y⟩ = |0⟩, we can discriminate the case \( N = 2 \) with input state \( |ψ⟩ = \frac{1}{\sqrt{2}}(|1⟩ + |2⟩) \). Furthermore, we can see in that oracle model, one-copy state can only discriminate one pair which is much less powerful than the one in our approach.

### B. Unentangled Discrimination Scheme

In the following we shall present a scheme of discrimination without any use of entanglement. In such scheme, the input state of \( t \)-copy network must be of the form

\[
|ψ⟩ = |ψ_1⟩ \otimes |ψ_2⟩ \otimes \cdots \otimes |ψ_t⟩
\]

(10)

Substitute the input state to the condition [3] for any pair \( (i, j) \), \( ⟨ψ_1|f_i^† f_j|ψ_1⟩⟨ψ_2|f_i^† f_j|ψ_2⟩\cdots⟨ψ_t|f_i^† f_j|ψ_t⟩ = 0 \). Thus, at least one block \( ⟨ψ_n|f_i^† f_j|ψ_n⟩ \) must be 0 in order to satisfy the equation. Namely the pair \((i,j)\) is discriminated by at least one \(|ψ_n⟩\).

In order to satisfy all the pairs in condition[5] any pair \((i,j)\) must be discriminated by at least one \(|ψ_n⟩\) in \( t \otimes |ψ_1⟩ \otimes |ψ_2⟩ \otimes \cdots \otimes |ψ_t⟩ \). A discrimination scheme is defined as a scheme to discriminate all the pairs in \( \{1, \ldots, N\} \) which are denoted as the set S_{alt} or K_{N}. We define the discrimination scheme with input state in the form of \(|ψ⟩ = |ψ_1⟩ \otimes |ψ_2⟩ \otimes \cdots \otimes |ψ_t⟩ \) as product discrimination scheme or unentangled discrimination scheme. Then for such scheme, it is required that \( U_{n=1}^t S_{|ψ_n⟩} = S_{alt} \).

It is interesting to find out the minimal \( t \) for any unentangled discrimination scheme. Any block \( ⟨ψ_n|f_i^† f_j|ψ_n⟩ \) which can not discriminate any pair namely trivial will not belong to the scheme due to the minimum copies requirement. We propose a product discrimination scheme with \( \frac{2}{3} N + 1 \) queries.

**Discrimination Scheme:** we construct the scheme only with \( < i, j > \) state. We divide all the \( N \) elements into groups, where each group contains 3 elements. Say the group of \( \{1,2,3\} \), we use \( < 1, 2 > \) and \( < 1, 3 > \) to discriminate all the pairs one of whose elements is in \( \{1,2,3\} \). It is easy to see we can use the same scheme.
for every group. If \( N \) elements cannot be divided into groups of 3 elements exactly, there is an incomplete group of 1 or 2 elements say \( \{N\} \) or \( \{N - 1, N\} \). We can use extra \( <1, N> \) or \( <1, N - 1> \) to discriminate the pairs which have one elements in the incomplete group. It is easy to verify that such a scheme is valid and use only at most \( \frac{2}{3}N + 1 \) copies.

However, it is surprising to see that such a simple scheme reaches the lower bound of product discrimination scheme. First, we will show it is sufficient to consider only 3 types states to simply our proof. A replacement of a block \( |\varphi\rangle \) by \( |\psi\rangle \) in unentangled discrimination scheme is valid if \( S_{|\varphi\rangle} \subseteq S_{|\psi\rangle} \). It is easy to see that such a replacement won’t diminish \( S_{|\psi\rangle} \) which guarantees the scheme after the replacement is also a valid discrimination scheme if it is before.

**Lemma 2.** For any unentangled discrimination scheme, if any block \( |\psi_n\rangle \) is not \( K_4 \) or \( <i, j> \) or \( E(i) \), we can always use a \( K_4 \) or \( <i, j> \) or \( E(i) \) to replace it validly.

**Proof:** The proof is a direct derivation of Lemma 2 because any block is a one-copy state. Using \( K_4 \) or \( <i, j> \) or \( E(i) \) to replace \( |\psi\rangle \) will guarantee the new set \( S \) contains \( S_{|\varphi\rangle} \). Therefore, we can replace validly. ■

Thus, directly by Lemma 2 we will only consider \( <i, j> \) or \( K_4 \) or \( E(i) \) as blocks in following discussion. However, due to the simplicity of analysis of the scheme when only \( <i, j> \) type states are in use, we seek to limit the number of other type states in the scheme. Therefore, it is natural to add an additional principle to the optimal scheme namely the more \( <i, j> \) states in use the better the same number of copies. We can always find such optimal scheme in all possible schemes with minimum number of copies, which means adding the new principle will not change the minimum number of copies for the problem. Finally, if we find in certain scheme we can use \( <i, j> \) states to replace other type states validly, such scheme must not be the optimal one in our principle. We can treat the replacement in two different ways. Firstly, a valid replacement is a indication that the current scheme is not optimal and may be out of our concerns. Secondly, a valid replacement can also be treated as a modification process to the optimal scheme. Sometimes, when a replacement of more than one block is necessary, the definition of validity is the natural extension of the one block case. This concept is important to understand the process of replacement in our following discussion.

Following the new principle, we want to obtain the property of the optimal discrimination scheme. It is easy to see the number of \( E(i) \) in the optimal scheme is at most 1. Otherwise, say there are two \( E(i) \) and \( E(j) \) in the optimal scheme, we can use \( <i, j> \) and \( <i, k> \) (any \( k \notin \{i, j\} \)) to replace them which contradicts its optimality. We denote a discrimination scheme using only \( <i, j> \) and \( K_4 \) as limited scheme. Let the number of copies in the optimal scheme be \( t_{opt} \) and the number in the optimal limited scheme be \( t'_{opt} \). If no \( E(i) \) appears in the optimal scheme, \( t_{opt} = t'_{opt} \). Otherwise, we can use \( <i, j> \) and \( <i, k> \) (any \( k \notin \{i, j\} \)) to replace \( E(i) \) and obtain \( t'_{opt} \leq t_{opt} + 1 \). Thus, \( t_{opt} \geq t'_{opt} - 1 \). The same idea will be used again once we bound the number of \( K_4 \) in the optimal limited scheme.

Next we shall seek for a lower bound of the limited scheme. For description simplicity, we use a graph language to depict the problem. We construct a graph \( G \) for any limited scheme in the following way. Each \( <i, j> \) or \( K_4 \) used in the scheme is treated as a type I or II vertex in the graph \( G \) respectively. There are only two types of edges in \( G \). If any two type I vertexes have a common element, there is an edge between them. For example, there is an edge between \( <i, j> \) and \( <i, k> \). If one type I vertex’s elements are included in a type II vertex, there is an edge between them. For example, there is an edge between \( <i, j> \) and \( K_4\{i, j, k, l\} \). It is easy and important to see for any \( <i, j> \), the pair \( (i, j) \) can be and only can be discriminated by the vertex adjacent to \( <i, j> \).

It should be noticed that the graph here is a representation of the discrimination scheme not the one we mention before to demonstrate the power of discrimination of each type state. In \( G \), we have \( t \) vertexes, \( l_1 \) type I and \( l_2 \) type II as well as many connected subgraphs \( \{G_n\} \). There are \( l_n \) vertexes in \( G_n \) in which \( l_1 \) type I and \( l_2 \) type II. Let \( D(G') = \{d_i|<d_{i1}, d_{i2}> \in G'\} \{e_i|<K_4\{e_i, e_i^2, e_i^3, e_i^4}\} \in G'\) for any graph \( G' \). Then it is important to see the following properties of the graph \( G \).

**Lemma 3.** For any optimal limited discrimination scheme, the corresponding graph \( G \) has following properties. The degree \( \Pi \) of any type II vertex is 0. For any subgraph \( G_n \) with at least one type I vertex, namely only type I vertex due to the claim above, \( l_n \geq 2 \) and \( |D(G_n)| \leq l_n + 1 \).

**Proof.** First, we can easily obtain that the degree of any type II vertex is at most 2. Assume we have a type II vertex with more than 2 adjacent vertexes(type I). Because \( K_4\{i, j, k, l\} \) has only 4 distinct elements, at least 2 of its adjacent vertexes have a common element, say \( <i, j> \) and \( <i, k> \). It is easy to see that such a \( K_4 \) is unnecessary because it can not discriminate any new pair. Thus, the only possible case where \( K_4\{a, b, c, d\} \) has degree 2 is its two adjacent vertexes must be \( <a, b> \) and \( <c, d> \). However, we can replace \( K_4\{a, b, c, d\} \) by \( <a, c> \) in such case. Therefore, degree 2 is also impossible for any type II vertex.

The type II vertex with degree 1 shares an edge with a type I vertex, say \( <i, j> \) and \( K_4\{i, j, k, l\} \), we can replace the \( K_4 \) by \( <i, k> \). Therefore no type II vertex with degree 1. Finally, the degree of any type II vertex is 0.

For any subgraph \( G_n \) with at least one type I vertex, it can only contain type I vertexes due to the result above. Any type I vertex \( <i, j> \) in \( G_n \) implies a need of an adjacent vertex to discriminate the pair \( (i, j) \). Thus \( l_n \geq 2 \). Any edge implies one repetition of appearance of the
common element and there are at least \( l_n - 1 \) edges in \( G_n \). Therefore, \( |D(G_n)| \leq 2l_n - (l_n - 1) = l_n + 1 \). 

It is only the case \( K_4 \) with degree 0 we have not discussed yet. Denote the set of all such type II vertex as \( G_K \). We have following lemma to bound \( |G_K| \). We define a pair is uniquely discriminated by a \( K_4 \) when no other vertex can discriminate the pair.

**Lemma 4.** \( |G_K| \leq 9 \).

**Proof.** Any \( K_4 \) in \( G_K \) must discriminate at least one pair uniquely. Due to our principle of preferring \( < i, j > \) to \( K_4 \), it is easy to check any vertex in \( G_K \) discriminates 1 or 2 pairs uniquely can always be replaced by \( < i, j > \) state. For the \( K_4 \) discriminating 3 pairs uniquely, only when it discriminates the pair \( (a, b), (a, c) \) and \( (b, c) \) (namely \( K_3(a, b, c) \)) it cannot be replaced. However, we will prove such \( K_4 \) will appear at most once. Once there are two such \( K_4 \), say \( K_4(a, b, c, d) \) and \( K_4(a', b', c', d') \), we can always replace them by two \( < i, j > \) type states. If \( \{a, b, c, d\} \cap \{a', b', c', d'\} = 3 \), say \( a, b, c \) are common elements, we can replace them by \( < a, b > \) and \( < c, c > \). Otherwise, \( \{a, b, c, d\} \cap \{a', b', c', d'\} \leq 2 \), because two \( K_4(a, b, c, d) \) and \( K_4(a', b', c', d') \) discriminates \( K_4(a, b, c) \) and \( K_3(a', b', c') \) uniquely, thus \( \{a, b, c\} \cap \{a', b', c'\} \leq 1 \) namely, at least two elements in one \( K_4 \) are different from the corresponding ones in another \( K_4 \), say \( b, b', c' \) are distinct. It should be noticed that to replace the two \( K_4 \), it is required that the new states can discriminate the pairs which are discriminated uniquely by the set \( K_4(a, b, c, d) \). If \( \{a, b, c, d\} \cap \{a', b', c', d'\} \leq 1 \), there is no pair discriminated by both \( K_4 \), then we can use \( < b, b' > \) and \( < c, c' > \) to replace the two \( K_4 \). If \( \{a, b, c, d\} \cap \{a', b', c', d'\} = 2 \), then \( \{a, d\} \) are common elements, we use \( < a, b > \) and \( < b, b' > \) instead. Finally, we obtain that all \( K_4 \) but at most one in \( G_K \) discriminate at least 4 pairs uniquely.

For any \( K_4(a, b, c, d) \) in \( G_K \), its 0 degree implies that once any element say \( a \) appears in any type I vertex, it must be \( < a, e > \) where \( e \notin \{a, b, c, d\} \). Namely, such \( < a, e > \) discriminates 3 pairs in \( \{a, b, c, d\} \) which makes \( K_4 \) fail to discriminate at least 4 pairs uniquely because \( K_4 \) can discriminate 6 pairs in total. Thus, all \( K_4 \) in \( G_K \) do not share elements with other type I vertex with at most one exception sharing 1 element. Therefore at least \( |D(G_K)| - 1 \) elements in \( D(G_K) \) won’t appear in \( D(G - G_K) \). Because any pair between these elements can only be discriminated by the vertex in \( G_K \). Then we have a necessary condition

\[
\frac{1}{2}(|D(G_K)| - 1)(|D(G_K)| - 2) \leq 6|G_K|.
\]

All \( K_4 \) in \( G_K \) can only discriminate pairs in \( D(G_K) \), which means all the pairs \( G_K \) can discriminate won’t exceed all the pairs in \( D(G_K) \). Thus we need \( |G_K| \leq \frac{2}{3}|D(G_K)| + 1 \), otherwise we can replace \( G_K \) by the discrimination scheme proposed at the beginning of the section using at most \( \frac{2}{3}|D(G_K)| + 1 \) copies. Combined with the inequality above, we have \( |D(G_K)| \leq 12 \) and \( |G_K| \leq \frac{2}{3}|D(G_K)| + 1 \leq 9 \).

In order to obtain a lower bound for the scheme, we need to have a necessary condition for a discrimination scheme as follows:

**Lemma 5.** For any limited discrimination scheme with corresponding graph \( G \), we have \( |D(G) \cap \{1, \ldots, N\}| \geq N - 1 \).

**Proof:** If there are at least two elements, say \( a \) and \( b \), are not in any \( \{d_1, d_2\} \) or \( K_4(e_1, e_2, e_3, e_4) \), then we cannot discriminate the pair \( (a, b) \) because this pair can only be discriminated by \( < a, c > \) or \( < b, c > \notin \{a, b\} \) state at least one of \( \{a, b\} \) will appear or by \( K_4(a, b, c, d) \) which both \( \{a, b\} \) will appear. Therefore, there is at most one element belonging to \( \{1, \ldots, N\} \) but not to \( D(G) \). Finally, we have \( |D(G) \cap \{1, \ldots, N\}| \geq N - 1 \).

**Theorem 1.** For any unentangled discrimination scheme with \( t \) copies, we have \( t \geq \frac{3}{2}N + c(N) \) asymptotically.

**Proof.** Because of Lemma 2, we have the optimal discrimination scheme can only use \( < i, j > \) or \( K_4 \) or \( E(i) \) state. We further seek for a lower bound of limited discrimination scheme. Due to Lemma 2, \( |G_K| \leq 9 \), we can replace each \( K_4(i, j, k, l) \) in \( G_K \) by \( < i, j > \) and \( < i, k > \) to make the scheme use only type I vertexes , using extra 9 copies. Using the same idea when we obtain \( t_{opt} \geq t_{opt}^1 - 9 \), denote the number of copies in the optimal scheme using only \( < i, j > \) as \( t_{opt}^2 \), we have \( t_{opt}^1 \geq t_{opt}^2 - 9 \) and \( t \geq t_{opt}^2 - 10 \).

Then we want to obtain \( t_{opt}^2 \). The new corresponding \( G \) has only type I vertexes and the analysis in Lemma 3 is also valid, we have \( |D(G_n)| \leq l_n + 1 = \alpha_n l_n \) where \( l_n \geq 2 \). Thus \( \alpha_n \leq \frac{2}{3} \) and \( |D(G_n)| \leq \frac{2}{3}l_n \).

\[
|D(G)| = \sum_{G_n} D(G_n) \leq \sum_{G_n} \sum_{G_n} \frac{3}{2}l_n = \frac{3}{2}t_{opt}^2
\]

Because of Lemma 5, \( |D(G)| \geq N - 1 \), we have \( t_{opt}^2 \geq \frac{3}{2}(N - 1) \) and finally \( t \geq t_{opt} \geq \frac{3}{2}N + c(N) \).

Finally, we prove \( \frac{3}{2}N \) is the asymptotic lower bound of the unentangled discrimination scheme. Combined with the discrimination scheme proposed at the beginning of the section, \( \frac{3}{2}N \) is also a tight lower bound.

It is interesting to see that using such unentangled discrimination scheme we can solve the Grover’s Oracle Identification Problem exactly using only \( \frac{3}{2}N + o(N) \) queries, which is less than \( N - 1 \) queries by a classical algorithm. We do not use entanglement which is considered to be the key role making quantum computing superior to classical one in the scheme. On the other side, only superposition and product state are used in the scheme. In the next section we shall consider the discrimination scheme where entanglement can be used.
C. Lower bound for a general parallel discrimination scheme

In order to achieve the general lower bound of such scheme, we first deal with the general structure of the input state of $t$ copies network. Recall the notation we use in Eq. (14) the general input state will be in following form $|\psi\rangle = \sum_{\vec{a}} p_{\vec{a}} |\vec{a}\rangle$. Let $\sigma$ be a permutation on $\vec{a}$, it is easy to verify that $\tau(\vec{a}) = \tau(\sigma(\vec{a}))$. Therefore, it’s reasonable to consider $\vec{a}$ only by the number of each label.

For any $\vec{a}$, let $c_i$ be the number of $a_k$ such that $a_k = i$, i.e., $c_i = \{|a_k| = i, 1 \leq k \leq t\}$. Obviously we have $\sum c_i = t$. Assume there are $l_1$ odd elements and $l_2$ even elements in $c_i$. For odd $c_i$, we have $c_i \geq 1$. Thus $l_1 \leq t$.

**Lemma 6.** Assume $t \leq \frac{N}{2}$. For any $\vec{a}$ with $\{c_i\}$ expression, the number of pairs $(i, j)$ which make $\tau(\vec{a})$ odd, denote as $n_{\vec{a}}$, is at most $t(N - t)$.

**Proof.** For any $\vec{a}$ with corresponding $\{c_i\}$ and any pair $(i, j)$, it is obvious that $\tau(\vec{a}) = c_i + c_j$. Thus, the total number of pairs $(i, j)$ that satisfy $\tau(\vec{a}) = 1$ is $l_1(N - l_1)$. Noting that $l_1 \leq t$ and $t \leq \frac{N}{2}$, we have $n_{\vec{a}} \leq t(N - t)$, the equality holds when $l_1 = t$.

The discriminating condition in Eq. (4) here becomes, for any pair $(i, j)$, $\sum_{\tau(\vec{a})=1} |p_{\vec{a}}|^2 - \sum_{\tau(\vec{a})=1} |p_{\vec{a}}|^2 = 0$. Because $\sum_{\vec{a}} |p_{\vec{a}}|^2 = 1$, we have

$$\sum_{\tau(\vec{a})=1} |p_{\vec{a}}|^2 = \frac{1}{2}. \quad (12)$$

**Theorem 2.** For any parallel discrimination scheme, the minimal number of copies for perfectly identifying Grover Oracle is not less than $\frac{1}{2}(N - \sqrt{N})$.

**Proof.** Without loss of generality, we may assume $t \leq N/2$. Otherwise the result automatically holds. Summing up Eq. (12) for all pairs $(i, j)$, we have:

$$\max_{\vec{a}}(n_{\vec{a}}) \sum_{\vec{a}} |p_{\vec{a}}|^2 \geq \sum_{\vec{a}} n_{\vec{a}} |p_{\vec{a}}|^2 = \frac{1}{4}N(N - 1). \quad (13)$$

If $t \leq \frac{N}{2}$, then it follows from Lemma 6 that $\max_{\vec{a}}(n_{\vec{a}}) \leq t(N - t)$. Thus we have

$$t(N - t) \geq \frac{1}{4}N(N - 1), \quad (14)$$

which together with the assumption $t \leq N/2$ implies that $t \geq \frac{1}{2}(N - \sqrt{N})$.

Although we don’t know whether the lower bound in the above theorem is tight, we do have found some interesting examples (in the next section) where the use of entanglement can dramatically reduce the number of the queries and meet this lower bound. So we believe that $\frac{1}{2}N$ queries is likely be saved by employing entanglement.

It has been shown that computing the boolean function OR is closely related to the unordered database search problem \[10\]. Clearly, an algorithm for computing OR function can also be used to do exact quantum search. The converse part, however, is not necessarily true. The complexity of computing OR function is in general higher than that of the exact quantum search. Our results are helpful in understanding such a difference. More precisely, in Ref. [11] it has been shown that $N$ requires is a tight lower bound for computing OR function, but here we have shown that $\frac{2}{3}N + 1$ is an upper bound for exact quantum search even in the absence of entanglement, and it is likely that such an upper bound can be reduced with the assistance of entanglement.

D. Some examples

We shall present several examples to demonstrate our results. We have analyzed the cases of $N = 2, 3, 4$ when we discuss the power of one-copy state. In this section we present two additional examples to demonstrate our results.

**Example 1.** It is easy to verify that when $N = 5$, it is impossible to identify unknown oracle with certainty by just one single use. Interestingly, there does exist a product discrimination scheme using just two queries. The input state is given as follows:

$$|\Phi_5\rangle = E(1) \otimes K_4\{2, 3, 4, 5\}, \quad (15)$$

where $E(1) = \frac{1}{\sqrt{3}}(1) + \frac{1}{\sqrt{3}}(2) + \frac{1}{\sqrt{3}}(3) + \frac{1}{\sqrt{3}}(4) + |5\rangle$ and $K_4\{2, 3, 4, 5\} = \frac{1}{\sqrt{3}}(2) + \frac{1}{\sqrt{3}}(3) + |4 \rangle + |5\rangle$.

The validity of the above scheme can be verified directly. Another way to see this is that $K_5$ is just covered by $S_{K_4(12, 3, 4)}$ and $S_{K_5(5)}$. We should point out that 2 queries is less than half of 5. That means its power beyond $\frac{1}{2}N$ lower bound.

However, we cannot solve the case of $N = 6$ using just two queries without the assistance of entanglement. Remarkably, by using an entangled state as input, we can achieve a perfect identification for the case $N = 6$.

**Example 2.** Take

$$|\Phi_6\rangle = \frac{1}{4}(\sum_{1 \leq i < j \leq 6} |ij\rangle + |33\rangle), \quad (16)$$

where $|33\rangle$ can be replaced by any $|kk\rangle$ such that $1 \leq k \leq 6$. We shall show that $f_k^{\otimes 2}|\Phi_6\rangle$ should be mutually orthogonal. A simple argument is as follows. It is clear that each $f_k^{\otimes 2}|\Phi_6\rangle$ contains exactly five terms with “+” sign. Taking inner product between $f_k^{\otimes 2}|\Phi_6\rangle$ and $f_l^{\otimes 2}|\Phi_6\rangle$, the sign before $|kl\rangle$ is changed into “+”, which results in a summation with 8 “+” signs. It follows from the lower bound $\frac{1}{2}(N - \sqrt{N})$ that two queries are optimal.
E. Solution to the general case

In the above, we completely analyzed the Grover’s Oracle Identification Problem which is a particular case of the unitary operation discrimination problem. Although the solution to the most general problem remains open, we can still make use of our techniques in the unentangled scheme to analyze some more general problems.

In our technique above, the distinction graph plays a very important role to understand the power of a state to discriminate unitary operations pair in the unentangled scheme. Also it is important for the possibility to employ graph and combinatorial skills in our analysis. For more general problem, such a distinction graph will also be helpful for our analysis.

One generalization of the current problem is to generalize the form of the oracle function \( f \). Namely, \( f \) can be any function mapping \( \{1,\ldots,N\} \) onto \( \{0,1\} \) and the quantum oracle is still the same form as the one in Eq. (4). In such case, the distinction graph and the latter combinatorial skills can still provide much help because of the fine discrete structure of such problems. However, when general unitary operations are considered, the distinction graph method might not be very efficient and powerful as before.

III. SUMMARY

In conclusion, we generalize the unsorted database search problem to the Grover’s Oracle Identification Problem which reveals both algorithmic and unitary operations distinguishing aspect of the problem and show the connection between them. In analysis, we obtain a tight lower bound \( \frac{2}{3} N \) for the product discrimination scheme and a general lower bound \( \frac{1}{2}(N-\sqrt{N}) \) for the parallel discrimination scheme. Finally, we also show that the complexity of exact quantum search with one unique solution can be strictly less than that of the calculation of OR function. Some interesting examples are also presented. Further more, we provide a brief idea to the solution with more general case.

There are still many interesting unsolved problems. For instance, we would like to know whether \( \frac{1}{2}(N-\sqrt{N}) \) is a tight lower bound for such scheme. Second, the lower bound for general unitary operation identification problem seems to be a great challenge.

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[18] \( \Omega(f(n)) \) means \( cf(n) \) where \( c \) is a positive constant.
[19] The degree of a vertex is the number of edges whose one end is the vertex.