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Additive composition formulation of the iterative Grover algorithm

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In the Grover-type quantum search process a search operator is iteratively applied, say, k times, on the initial uniform superposition database state. We present an additive decomposition scheme such that the iteration process is expressed, in the computational space, as a linear combination of k operators, each of which consists of a single Grover-search followed by an overall phase-rotation. The value of k and the rotation phase are the same as those determined in the framework of the search with certainty. We discuss how the additive form can be effectively utilized and we propose an alternative gate that realizes the same outcome as the iterative search.

I. INTRODUCTION

In the Grover-type quantum search process [1–6] a search operator is iteratively applied on the initial database state that consists of $N = 2^n$ unordered basis states to search for M target states, n being the number of qubit-registers. The phase matching method [7–9, 11–13] for the Grover quantum search algorithm has been extensively studied and shown to be effective in improving the success probability $P_k(\lambda)$, where $\lambda = M/N$ is the ratio of the number of target states to the number of database states and k is the number of iterations. In spite of the impressive efficacy of this method for most values of λ , it is less so when $\lambda \ll 1$.

In Ref. [7], we investigated the problem of an exact search with the success probability $P_k(\lambda) = 1$ for any value of λ , on the basis of the phase-matched search-operator $G_N(\alpha) \equiv W_N(-\alpha)U_N(\alpha)$, where $U_N(\alpha)$ is the oracle operator, $W_N(-\alpha)$ is the diffusion operator and α is the matching phase. The search operator originally used by Grover is a special case with $\alpha = \pi$. We assumed that λ is known preliminarily. Then the phase matching method enabled us to accomplish an exact search. We gave analytic forms of the optimal number of searches k and the matching phase α_k for an exact search for the entire range of $0 < \lambda \leq 1$. We showed that $k = k_G$ or $k = k_G + 1$, where k_G is the optimal number of searches of the original Grover algorithm (see Fig. 1 of Ref. [7]). Recall that, in the original version of the Grover search, $P_{k_G}(\lambda) = 1$ can be satisfied only for $\lambda = 1/4$ and $\lambda = 1$ [14][20]. The modification of the Grover algorithm to obtain zero failure by means of a phase rotation was first suggested by Long [10].

The purpose of this paper is to propose an alternative search process. We first derive, in the N -dimensional computational space, an additive decomposition scheme for the k -iterative search state $|\phi_k\rangle = G_N^k(\alpha)|\phi_0\rangle$, where $|\phi_0\rangle$ and $|\phi_k\rangle$ are respectively the initial database state and the final state. The decomposed form includes a linear combination of k components each of which consists of a single Grover-search operator $G_N(\alpha)$ followed by an overall phase-rotation. The phase-rotation parameter is determined by α and λ , or by the optimal number of iterations k for the exact search. The phase-rotation parameter can be determined preliminarily. In the decomposed form, $|\phi_k\rangle$ can be expressed as a simple superposition of $|\phi_0\rangle$ and $|\phi_1\rangle$ with superposition coefficients that are determined by the phase-rotation parameter. This enables us to obtain $|\phi_k\rangle$ with only the information of $|\phi_1\rangle$. Furthermore, it is noteworthy that $|\phi_1\rangle$ can be expressed in terms of only the oracle operation $U_N(-\alpha)|\phi_0\rangle$ and the phase-rotation parameter, without the diffusion operator $W_N(\alpha)$. Thus we obtain $|\phi_k\rangle$ as an expression consisting of terms linear in $U_N(-\alpha)$ and functions of the phase-rotation parameter. This is a key feature of the additive decomposition scheme.

As we show in due course, however, the reduced operator itself obtained in the decomposition is, unlike $G_N^k(\alpha)$, not unitary except in the case of $n = 1$ ($N = 2$), although the norm of $|\phi_k\rangle$ is preserved in the decomposition. By making use of the reduced form for $|\phi_k\rangle$ and on the basis of the search-with-certain-outcome algorithm [7], however, we can define a unitary gate that directly transforms $|\phi_0\rangle$ to $|\phi_k\rangle$. The unitary transformation from $|\phi_0\rangle$ to $|\phi_k\rangle$ provides an alternative to the Grover-type iterative searches. The unitary transformation so obtained is much simpler than the corresponding k -iterative search operator $G_N^k(\alpha)$. We will show this by examining the matrix representations of the new operator and the iterative search operator $G_N^k(\alpha)$.

In Sec. II, we first give a brief review of the exact search algorithm that was developed in Ref. [7] and subsequently derive the decomposition scheme. In Sec. III, we present an alternative scheme for the iterative search in the framework of the exact search. Section IV contains a summary. In Appendix A we give an illustration of the decomposition scheme.

II. ADDITIVE DECOMPOSITION SCHEME OF AN ITERATIVE SEARCH ALGORITHM

A. Iterative-search with $P_k(\lambda) = 1$ for $0 < \lambda \leq 1$

We first give a brief review of the iterative search algorithm that yields exactly $P(\lambda) = 1$ for any $0 < \lambda (= M/N) \leq 1$ [7]. In the computational space of $N = 2^n$ dimensions, a modified Grover algorithm based on the phase matching method is represented by the oracle operator $U_N(\alpha)$ and the diffusion operator $W_N(-\alpha)$,

$$U_N(\alpha) = I_N - (1 - e^{i\alpha}) \sum_{l=0}^{M-1} |t_l\rangle\langle t_l|, \quad (1)$$

$$\begin{aligned} W_N(-\alpha) &= H^{\otimes n} [I_N e^{-i\alpha} + (1 - e^{-i\alpha}) |0^{\otimes n}\rangle\langle 0^{\otimes n}|] H^{\otimes n} \\ &= I_N e^{-i\alpha} + (1 - e^{-i\alpha}) |\phi_0\rangle\langle \phi_0|, \end{aligned} \quad (2)$$

where α is the matching phase, suffix N indicates that the operators are of the computational space, $|0^{\otimes n}\rangle$ is the n -qubit initialized register state and H is the Walsh-Hadamard transformation. The unstructured initial database state $|\phi_0\rangle$ is defined by $|\phi_0\rangle = H^{\otimes n}|0^{\otimes n}\rangle = (1/\sqrt{N}) \sum_{l=0}^{N-1} |\omega_l\rangle$, where $|\omega_l\rangle$ are the computational basis states. The $|\phi_0\rangle$ can also be written as $|\phi_0\rangle = \sqrt{1-\lambda}|R\rangle + \sqrt{\lambda}|T\rangle$, where $|T\rangle$ is the uniform superposition of target states $|t_l\rangle$, i.e., $|T\rangle = \frac{1}{\sqrt{M}} \sum_{l=0}^{M-1} |t_l\rangle$, and $|R\rangle$ is that of the remaining states $|r_l\rangle$, i.e., $|R\rangle = \frac{1}{\sqrt{N-M}} \sum_{l=0}^{N-M-1} |r_l\rangle$.

A k -iterative search is done by k iterative operations of the kernel operator $G_N(\alpha) \equiv W_N(-\alpha)U_N(\alpha)$ on $|\phi_0\rangle$, i.e.,

$$|\phi_k\rangle = G_N^k(\alpha)|\phi_0\rangle, \quad (3)$$

where $|\phi_k\rangle$ is the state obtained by the k iterative search. In Ref. [7], we showed that the matching phase α for the exact search with $P_k(\lambda) = 1$ can be determined in terms of λ and k as

$$\alpha_k(\lambda) = \arccos \left[1 - \frac{1 - \cos(\pi/(2k+1))}{\lambda} \right]. \quad (4)$$

For a given value of λ , we first determine the optimal number k of the iterations as the smallest integer that is compatible with

$$k \geq \frac{\pi - \arccos(1 - 2\lambda)}{2 \arccos(1 - 2\lambda)}. \quad (5)$$

The optimal k is a staircase function of λ (see Fig. 1 of Ref. [7]). If we know λ preliminarily, by using Eqs. (4) and (5) we can determine the optimal k and $\alpha_k(\lambda)$ for the search with certainty. As mentioned in the introduction, the optimal k for the exact search is always equal to, or greater by one than, that of the original Grover search depending on the value of λ .

B. Novel relation between $G_N(\alpha)$ and $G_N^\dagger(\alpha)$

We present a useful relationship between $G_N(\alpha)$ and $G_N^\dagger(\alpha)$ for the purpose of applying it to the decomposition scheme for the iterative search mentioned in the previous sub-section. By using Eqs. (1) and (2), it can be verified that the initial state $|\phi_0\rangle$ is an eigenstate of $G_N(\alpha) + G_N^\dagger(\alpha)$ with the eigenvalue $\epsilon = 2[1 - \lambda(1 - \cos \alpha)]$, namely

$$[G_N(\alpha) + G_N^\dagger(\alpha)] |\phi_0\rangle = \epsilon |\phi_0\rangle = 2[1 - \lambda(1 - \cos \alpha)] |\phi_0\rangle. \quad (6)$$

In fact, $|T\rangle$ and $|R\rangle$ are individually eigenstates of $G_N(\alpha) + G_N^\dagger(\alpha)$ belonging to the same eigenvalue ϵ .

First, we show that ϵ is equal to the trace of the search operator $G_{[2]}(\alpha) \equiv W_{[2]}(-\alpha)U_{[2]}(\alpha)$ represented in the two-dimensional space spanned by the basis $\{|R\rangle, |T\rangle\}$. In this space the search operator $G_{[2]}(\alpha)$ is [7],

$$G_{[2]}(\alpha) = \begin{pmatrix} 1 - (1 - e^{-i\alpha})\lambda & - (1 - e^{i\alpha})\sqrt{\lambda(1-\lambda)} \\ (1 - e^{-i\alpha})\sqrt{\lambda(1-\lambda)} & 1 - (1 - e^{i\alpha})\lambda \end{pmatrix}. \quad (7)$$

It turns out that $\text{Tr}G_{[2]}(\alpha) = 2[1 - \lambda(1 - \cos \alpha)] = \epsilon_+ + \epsilon_- = \epsilon$, where $\epsilon_{\pm}$ are the two eigenvalues of $G_{[2]}(\alpha)$. The $\epsilon_{\pm}$ are given by

$$\epsilon_{\pm} = 1 - \lambda(1 - \cos \alpha) \pm i\sqrt{\lambda(1 - \cos \alpha)[2 - \lambda(1 - \cos \alpha)]}. \quad (8)$$

Since $G_{[2]}(\alpha)$ is unitary, of course $|\epsilon_{\pm}| = 1$. The two eigenvalues ϵ_+ and ϵ_- are complex conjugate of each other and satisfy the relation $\epsilon_+\epsilon_- = 1$. We can express $\epsilon_{\pm}$ as $\epsilon_{\pm} = e^{\pm i\theta}$, where

$$\theta = \arctan\left(\frac{\sqrt{x(2-x)}}{1-x}\right), \quad x \equiv \lambda(1 - \cos \alpha). \quad (9)$$

From (8), it is seen that the phase θ is simply related to α and λ as,

$$\cos \theta = 1 - \lambda(1 - \cos \alpha). \quad (10)$$

Equation (6) can be rewritten as

$$[G_N(\alpha) + G_N^{\dagger}(\alpha)]|\phi_0\rangle = (\epsilon_+ + \epsilon_-)|\phi_0\rangle = (e^{i\theta} + e^{-i\theta})|\phi_0\rangle. \quad (11)$$

It should be stressed that (11) holds as an eigenvalue equation. On the other hand, in the two-dimensional representation of (7), the relation $G_{[2]}(\alpha) + G_{[2]}^{\dagger}(\alpha) = [\text{Tr}G_{[2]}(\alpha)]I_2 = (\epsilon_+ + \epsilon_-)I_2$ holds as a relation between the two-dimensional unitary matrices $G_{[2]}(\alpha)$ and $G_{[2]}^{\dagger}(\alpha)$. This relation can be proved by using the two dimensional Cayley-Hamilton theorem for unitary $G_{[2]}(\alpha)$ with its $\det G_{[2]}(\alpha) = 1$.

Next, we extend the relation (11) to an arbitrary number of searches k . By operating $G_N(\alpha) + G_N^{\dagger}(\alpha)$ on both sides of (11) from the left, we obtain,

$$\left\{G_N(\alpha)^2 + [G_N^{\dagger}(\alpha)]^2 + 2I_N\right\}|\phi_0\rangle = (\epsilon_+ + \epsilon_-)[G_N(\alpha) + G_N^{\dagger}(\alpha)]|\phi_0\rangle = (\epsilon_+ + \epsilon_-)^2|\phi_0\rangle, \quad (12)$$

where the unitarity of $G_N(\alpha)$ was used. Equation (12) can be rewritten as

$$\left\{G_N^2(\alpha) + [G_N^{\dagger}(\alpha)]^2\right\}|\phi_0\rangle = [(\epsilon_+ + \epsilon_-)^2 - 2]|\phi_0\rangle = (\epsilon_+^2 + \epsilon_-^2)|\phi_0\rangle, \quad (13)$$

where $\epsilon_+\epsilon_- = 1$ was used. Since $[G_N^{\dagger}(\alpha)]^2 = [G_N^2(\alpha)]^{\dagger}$ we obtain,

$$\left\{G_N^2(\alpha) + [G_N^2(\alpha)]^{\dagger}\right\}|\phi_0\rangle = (\epsilon_+^2 + \epsilon_-^2)|\phi_0\rangle. \quad (14)$$

By repeating the same procedure, we obtain

$$\left\{G_N^k(\alpha) + [G_N^k(\alpha)]^{\dagger}\right\}|\phi_0\rangle = (\epsilon_+^k + \epsilon_-^k)|\phi_0\rangle = (e^{ik\theta} + e^{-ik\theta})|\phi_0\rangle \quad (15)$$

for any number k of searches. For $k = 0$, (15) should be understood as $(I_N + I_N^{\dagger})|\phi_0\rangle = (\text{Tr}I_2)|\phi_0\rangle = 2|\phi_0\rangle$. The decomposition scheme presented in this subsection holds for any search specified by k , N and λ , as long as θ is determined by the relation (10). The search does not always have to be the exact search of Ref. [7] reviewed in subsection II A.

For the exact search of Ref. [7], $\alpha_k(\lambda)$ is given by (4). In this case, from (4) and (10) it turns out that the phase θ_k is determined by the optimal k alone as

$$\theta_k = \frac{\pi}{2k+1}. \quad (16)$$

Since the optimal k is a staircase function of λ , so is θ_k .

C. Additive decomposition scheme of $G_N^k(\alpha)|\phi_0\rangle$

We now construct the decomposition scheme on the basis of (15). By applying $G_N^k(\alpha)$ to the left of both sides of (15), we obtain,

$$[G_N^{2k}(\alpha) + I_N] |\phi_0\rangle = (e^{ik\theta} + e^{-ik\theta}) G_N^k(\alpha) |\phi_0\rangle. \quad (17)$$

Equation (17) can be rewritten as

$$\begin{aligned} |\phi_{2k}\rangle &\equiv G_N^{2k}(\alpha) |\phi_0\rangle = [(e^{ik\theta} + e^{-ik\theta}) G_N^k(\alpha) + e^{i\pi} I_N] |\phi_0\rangle \\ &\equiv e^{ik\theta} |\phi_k\rangle + e^{-ik\theta} |\phi_k\rangle + e^{i\pi} |\phi_0\rangle. \end{aligned} \quad (18)$$

Equation (18) implies that the $2k$ search can be decomposed into a sum of two k -iterative searches, $e^{ik\theta} G_N^k(\alpha) |\phi_0\rangle$ and $e^{-ik\theta} G_N^k(\alpha) |\phi_0\rangle$, and a constant phase transformation $e^{i\pi} I_N |\phi_0\rangle$. The first two operations consist of k searches of $G_N^k(\alpha)$ followed by the unitary overall phase rotation $e^{\pm ik\theta} I_N = e^{\pm ik\theta} I_2^{\otimes n}$. With the aid of (15), it can directly be confirmed that the norm of the decomposed form $e^{ik\theta} |\phi_k\rangle + e^{-ik\theta} |\phi_k\rangle + e^{i\pi} |\phi_0\rangle$ is unity, where the norm of $|\phi_k\rangle$ is of course unity. Equation (18) gives a basic decomposition scheme for an even number of iterations.

By operating $G_N(\alpha)$ on (18) from the left, a basic decomposition scheme for an odd number of iterations is obtained as

$$\begin{aligned} |\phi_{2k+1}\rangle &\equiv G_N^{2k+1}(\alpha) |\phi_0\rangle = G_N(\alpha) (e^{ik\theta} |\phi_k\rangle + e^{-ik\theta} |\phi_k\rangle + e^{i\pi} |\phi_0\rangle) \\ &\equiv e^{ik\theta} |\phi_{k+1}\rangle + e^{-ik\theta} |\phi_{k+1}\rangle + e^{i\pi} |\phi_1\rangle. \end{aligned} \quad (19)$$

Similarly to the case of an even number of iterations of (18), it can directly be confirmed that the norm of the decomposed expression $e^{ik\theta} |\phi_{k+1}\rangle + e^{-ik\theta} |\phi_{k+1}\rangle + e^{i\pi} |\phi_1\rangle$ is unity, where the norms of $|\phi_{k+1}\rangle$ and $|\phi_1\rangle$ are both unity.

By using the two basic decomposition schemes of (18) and (19), we can decompose a search of any number of iterations into a linear combination of a single Grover search operator followed by overall phase rotations of the form of $e^{\pm im\theta} I_N$ (m : an integer) and a constant phase rotation $e^{i\pi} I_N$. We give below explicit forms of the decompositions for the first three values of k

$$|\phi_1\rangle = G_N(\alpha) |\phi_0\rangle = [(e^{i\theta} + e^{-i\theta}) I_N + e^{i\pi} G_N^\dagger(\alpha)] |\phi_0\rangle, \quad (20)$$

$$|\phi_2\rangle = G_N^2(\alpha) |\phi_0\rangle = [(e^{i\theta} + e^{-i\theta}) G_N(\alpha) + e^{i\pi} I_N] |\phi_0\rangle, \quad (21)$$

$$|\phi_3\rangle = G_N^3(\alpha) |\phi_0\rangle = [(e^{2i\theta} + e^{-2i\theta} + 1) G_N(\alpha) + (e^{i\theta} + e^{-i\theta}) e^{i\pi} I_N] |\phi_0\rangle, \quad (22)$$

For $k \geq 2$, it is seen by induction, that the additive decomposition of $|\phi_k\rangle$ can be summarized as,

$$|\phi_k\rangle = G_N^k(\alpha) |\phi_0\rangle = [f_k(\theta) G_N(\alpha) + f_{k-1}(\theta) e^{i\pi} I_N] |\phi_0\rangle \equiv G_N^{I,k}(\theta, \alpha) |\phi_0\rangle, \quad (23)$$

where $G_N^{I,k}(\theta, \alpha) \equiv f_k(\theta) G_N(\alpha) + f_{k-1}(\theta) e^{i\pi} I_N$, and $f_k(\theta)$ is given as,

$$f_0(\theta) = 0, \quad f_1(\theta) = 1, \quad f_k(\theta) = f_{k-1}(\theta) (e^{i\theta} + e^{-i\theta}) - f_{k-2}(\theta) \quad \text{for } k \geq 2. \quad (24)$$

Note that $f_k^*(\theta) = f_k(\theta)$. The norm of the reduced form of $G_N^{I,k}(\theta, \alpha) |\phi_0\rangle$ of (23) again can be verified to be unity for any k with the aid of the relation $[G_N(\alpha) + G_N^\dagger(\alpha)] |\phi_0\rangle = (e^{i\theta} + e^{-i\theta}) |\phi_0\rangle$ of (11) and the identity $f_{k-1}^2(\theta) - f_k(\theta) f_{k-2}(\theta) = 1$ which follows from (24). Only when $N = 2$, $G_N^{I,k}(\theta, \alpha)$ is unitary.

As seen in (20), $|\phi_1\rangle = G_N(\alpha) |\phi_0\rangle$ can also be expressed in terms of $G_N^\dagger(\alpha)$ instead of $G_N(\alpha)$. Equation (20) can further be rewritten as

$$\begin{aligned} |\phi_1\rangle &= G_N(\alpha) |\phi_0\rangle = [(e^{i\theta} + e^{-i\theta}) I_N + e^{i\pi} G_N^\dagger(\alpha)] |\phi_0\rangle \\ &= (f_2(\theta) I_N + e^{i\pi} U_N(-\alpha)) |\phi_0\rangle, \end{aligned} \quad (25)$$

where the relation $G_N^\dagger(\alpha) |\phi_0\rangle = U_N^\dagger(\alpha) W_N^\dagger(-\alpha) |\phi_0\rangle = U_N(-\alpha) W_N(\alpha) |\phi_0\rangle = U_N(-\alpha) |\phi_0\rangle$ was used. Here, note that $W_N(\alpha) |\phi_0\rangle = |\phi_0\rangle$. Thus, in order to obtain $|\phi_1\rangle$ we need only the oracle operation $U_N(-\alpha) |\phi_0\rangle$. By using $|\phi_1\rangle$ of

(28) in (26), we can express $|\phi_k\rangle$ as

$$\begin{aligned} |\phi_k\rangle &= [(f_k(\theta)f_2(\theta) + e^{i\pi}f_{k-1}(\theta))I_N + e^{i\pi}f_k(\theta)U_N(-\alpha)]|\phi_0\rangle \\ &= [g_k(\theta)I_N + h_k(\theta)U_N(-\alpha)]|\phi_0\rangle, \\ &\equiv G_N^{II,k}(\theta, \alpha)|\phi_0\rangle, \end{aligned} \quad (26)$$

where $G_N^{II,k}(\theta, \alpha) \equiv g_k(\theta)I_N + h_k(\theta)U_N(-\alpha)$, $g_k(\theta) \equiv f_k(\theta)f_2(\theta) + e^{i\pi}f_{k-1}(\theta)$ and $h_k(\theta) \equiv e^{i\pi}f_k(\theta)$. Thus $|\phi_k\rangle$ can be obtained by an operator acting on $|\phi_0\rangle$ which consists of k terms involving the oracle operation $U_N(-\alpha)$ times a phase factor as well as phase factors terms. No diffusion operation is needed to obtain $|\phi_k\rangle$. This is a key feature of the additive decomposition of the iterative search process. As the diffusion operator is eliminated from $G_N^{I,k}(\theta, \alpha)$ of (23) by using $W_N(\alpha)|\phi_0\rangle = |\phi_0\rangle$, $G_N^{II,k}(\theta, \alpha)$ is no longer unitary even for $N = 2$. Note that for the exact search $g_k(\theta_k) + h_k(\theta_k) = 0$ holds with $\theta_k = \pi/(2k+1)$.

The identity for $|\phi_k\rangle$ of (23) (or (26)) holds for any search specified by k , N and λ , as long as θ is determined by the relation (10). The additive form (26) is especially useful in obtaining the vector-component representation of $|\phi_k\rangle$. For example, when the targets are the first M states $|\omega_0\rangle, \dots, |\omega_{M-1}\rangle$, by using (26) we can write $|\phi_k\rangle$ at first sight as,

$$|\phi_k\rangle = (\overbrace{v_t, \dots, v_t}^M, \overbrace{v_{nt}, \dots, v_{nt}}^{N-M})^T, \quad (27)$$

where T indicates *transposed* and v_t and v_{nt} are respectively the amplitude of the target states and the non-target states. By using (29), the amplitudes v_t and v_{nt} are immediately obtained as,

$$v_t = \frac{1}{\sqrt{N}} [g_k(\theta) + h_k(\theta)e^{-i\alpha}], \quad (28)$$

$$v_{nt} = \frac{1}{\sqrt{N}} [g_k(\theta) + h_k(\theta)]. \quad (29)$$

In Ref. [7], we presented compact forms of the success and failure amplitudes, i.e., d_k and u_k respectively,

$$d_k = \frac{\sqrt{\lambda}}{\sin(\theta/2)} \left\{ \sin \left[\left(k + \frac{1}{2} \right) \theta \right] - \frac{(1 + e^{-i\alpha}) \sin(k\theta)}{2 \cos(\theta/2)} \right\} \quad (30)$$

$$u_k = \frac{\sqrt{1-\lambda}}{\cos(\theta/2)} \cos \left[\left(k + \frac{1}{2} \right) \theta \right]. \quad (31)$$

These amplitudes are defined in the two-dimensional space spanned by $\{|R\rangle, |T\rangle\}$. It can be verified that the relations $\sqrt{M}v_t = d_k$ and $\sqrt{N-M}v_{nt} = u_k$ hold.

In the exact search with $P_k(\lambda) = 1$ for a given λ , the optimal k , $\alpha_k(\lambda)$ and θ_k are respectively determined by (5), (4) and (16) (or (10)). With these values of k , α_k and θ_k , $M|v_t|^2 = 1$ and $v_{nt} = 0$.

Before ending this section, we have to stress the following point. Equation (23) (or (26)) is an identity for the final state $|\phi_k\rangle$. In Appendix A, we illustrate this situation for the case of $n = 3$ ($N = 8$) and the target $|t_0\rangle = |000\rangle$. In this case, the optimal number of searches is $k = 2$ since $\lambda = 1/8$. From (A.4) and (A.7), it will be seen that (21) (or (23)) is a correct identity for $|\phi_2\rangle$, where the phase parameter θ_2 contains the information on the two iterations.

On the other hand, the following point is especially crucial. Although the reduced operator $G_N^{I,k}(\theta, \alpha)$ of (23) yields $|\phi_k\rangle$, $G_N^{I,k}(\theta, \alpha)$ itself is not unitary except in the trivial case of $n = 1$ ($N = 2$). Therefore $G_N^{I,k}(\theta, \alpha)$ cannot in general be interpreted as a quantum mechanical evolution operator. The reason is as follows. In order to validate the unitarity of $G_N^{I,k}(\theta, \alpha)$, we need the relation $G_N(\alpha) + G_N^\dagger(\alpha) = (e^{i\theta} + e^{-i\theta})I_N$ for the two unitary operators $G_N(\alpha)$ and $G_N^\dagger(\alpha)$. This relation holds only for the $N = 2$ ($n = 1$) case. For $N > 2$, however, it does not hold. On the other hand, the eigenvalue equation $[G_N(\alpha) + G_N^\dagger(\alpha)]|\phi_0\rangle = (e^{i\theta} + e^{-i\theta})|\phi_0\rangle$ is valid for any N , which guarantees that the norm of $G_N^{I,k}(\theta, \alpha)|\phi_0\rangle$ is unity. This is why (23) is an identity for $|\phi_k\rangle$.

III. CONSTRUCTION OF A UNITARY TRANSFORMATION SUGGESTED BY THE ADDITIVE DECOMPOSITION

In this section we discuss a possible scheme suggested by the additive decomposition scheme and construct a unitary transformation on the basis of the reduced form of (26). As mentioned at the end of sub-section II C, although the

k -iterative search operator $G_N^k(\alpha)$ can be realized as a quantum-mechanical evolution-operator, the reduced operator $G_N^{II,k}(\theta, \alpha) = [g_k(\theta)I_N + h_k(\theta)U_N(-\alpha)]$ of (26) cannot be interpreted as a quantum mechanical evolution in general, even though $G_N^{II,k}(\theta, \alpha)|\phi_0\rangle$ is identical to $G_N^k(\alpha)|\phi_0\rangle$. The advantage of $G_N^{II,k}(\theta, \alpha)$ is that it allows us to obtain $|\phi_k\rangle$ with an operator including only k terms involving the linear form of $U_N(-\alpha)$, where the information on the k -iterative search is provided by θ . No diffusion operation is needed. This is a remarkable point. In what follows, we discuss how we can take advantage of $G_N^{II,k}(\theta, \alpha)$ to construct a unitary operator that functions as the search operator.

According to (26), the final search state $|\phi_k\rangle = G_N^{II,k}(\theta, \alpha)|\phi_0\rangle$ is given as a superposition of the initial state $|\phi_0\rangle$ and the state obtained by one-oracle operation $|\phi_U\rangle \equiv U_N(-\alpha)|\phi_0\rangle$. The superposition coefficients $g_k(\theta)$ and $h_k(\theta)$ are basically sums of phase rotations $e^{\pm im\theta}$ and $e^{i\pi}$. Figure 1 shows a unitary processing scheme utilizing the reduced form of (26). It is understood that the superposition coefficients $g_k(\theta)$ and $h_k(\theta)$ are incorporated in the additive transformation C_N .

FIG. 1: (Colour online) A unitary processing scheme utilizing the reduced form of (26), $G_N^{II,k}(\theta_k, \alpha_k)|\phi_0\rangle = [g_k(\theta_k)I_N + h_k(\theta_k)U_N(-\alpha_k)]|\phi_0\rangle \equiv g_k(\theta_k)|\phi_0\rangle + h_k(\theta_k)|\phi_U\rangle$, where $|\phi_U\rangle \equiv U_N(-\alpha_k)|\phi_0\rangle$, and k, α_k and θ_k are those for a certain search. The unitary transformation $C_N(k, \theta_k, \alpha_k; |\omega_i\rangle, \dots)$ incorporates the reduced operator $G_N^{II,k}(\theta_k, \alpha_k)$.

We now consider a certain search with λ given in advance so that the optimal k , α_k , and θ_k for the certain search are determined from (5), (4), and (16), respectively. The unitary processing scheme shown in Fig. III is then written as,

$$|\phi_k\rangle = C_N(k, \theta_k, \alpha_k; |\omega_i\rangle, \dots)|\phi_0\rangle. \quad (32)$$

The unitary operator C_N is systematically constructed as follows. First, we prepare two orthonormal sets $\{|\phi_k^{(0)}\rangle \equiv |\phi_k\rangle, |\phi_k^{(1)}\rangle, \dots, |\phi_k^{(N-1)}\rangle\}$ and $\{|\phi_0^{(0)}\rangle \equiv |\phi_0\rangle, |\phi_0^{(1)}\rangle, \dots, |\phi_0^{(N-1)}\rangle\}$. With these orthonormal stets, the unitary operator C_N in (32) is constructed as,

$$C_N(k, \theta_k, \alpha_k; |\omega_i\rangle, \dots) = \underline{|\phi_k^{(0)}\rangle\langle\phi_0^{(0)}|} + |\phi_k^{(1)}\rangle\langle\phi_0^{(1)}| + \dots + |\phi_k^{(N-1)}\rangle\langle\phi_0^{(N-1)}|, \quad (33)$$

where the underlined term $|\phi_k^{(0)}\rangle\langle\phi_0^{(0)}| = |\phi_k\rangle\langle\phi_0|$ realizes the transformation defined in (32) and the other terms are needed for the unitarity of C_N . We discuss (33) more explicitly in the following.

To make the point clearer, we first consider the case of a single target, i.e., $|t\rangle = |\omega_i\rangle$ ($i = 0, \dots, N-1$). In this case, from (26) $|\phi_k\rangle = G_N^{II,k}(\theta_k, \alpha_k; |\omega_i\rangle)|\phi_0\rangle = [g_k(\theta_k)I_N + h_k(\theta_k)U_N(-\alpha_k; |\omega_i\rangle)]|\phi_0\rangle = v_t|\omega_i\rangle$ with $|v_t| = 1$. The C_N is then written as,

$$\begin{aligned} C_N(k, \theta_k, \alpha_k; |\omega_i\rangle) &= \underline{G_N^{II,k}(\theta_k, \alpha_k; |\omega_i\rangle)|\phi_0\rangle\langle\phi_0|} + \sum_{j=0(\neq i), l=1}^{N-1} G_N^{II,k}(\theta_k, \alpha_k; |\omega_j\rangle)|\phi_0\rangle\langle\phi_0^{(l)}| \\ &= v_t \left[\underline{|\omega_i\rangle\langle\phi_0|} + \sum_{j=0(\neq i), l=1}^{N-1} |\omega_j\rangle\langle\phi_0^{(l)}| \right]. \quad (i = 0, \dots, N-1) \end{aligned} \quad (34)$$

It should be noted that there is an ambiguity in choosing the combination $|\omega_j\rangle$ ($j \neq i$) and $\langle\phi_0^{(l)}|$ ($l \neq 0$). The initial

state $|\phi_0\rangle$ is $H^{\otimes n}|0^{\otimes n}\rangle$. Therefore, the orthonormal set $\{|\phi_0\rangle, |\phi_0^{(1)}\rangle, \dots, |\phi_0^{(N-1)}\rangle\}$ are, for example, taken as

$$|\phi_0\rangle = H^{\otimes n}|0\rangle^{\otimes n} = H|0\rangle \otimes \dots \otimes H|0\rangle \otimes H|0\rangle \quad (35)$$

$$|\phi_0^{(1)}\rangle = (I_2 \otimes \dots \otimes I_2 \otimes \sigma_z) |\phi_0\rangle = H|0\rangle \otimes \dots \otimes H|0\rangle \otimes \sigma_z H|0\rangle \quad (36)$$

$$|\phi_0^{(2)}\rangle = (I_2 \otimes \dots \otimes \sigma_z \otimes I_2) |\phi_0\rangle = H|0\rangle \otimes \dots \otimes \sigma_z H|0\rangle \otimes H|0\rangle \quad (37)$$

$$\vdots$$

$$|\phi_k^{(N-1)}\rangle = (\sigma_z \otimes \dots \otimes \sigma_z \otimes \sigma_z) |\phi_0\rangle = \sigma_z H|0\rangle \otimes \dots \otimes \sigma_z H|0\rangle \otimes \sigma_z H|0\rangle, \quad (38)$$

where H and σ_z are respectively the Hadamard and Pauli gate. With this choice of $|\phi_0^{(i)}\rangle$, for example, for an assumed single target $|t\rangle = |\omega_0\rangle$, C_N of (34) is more explicitly given as,

$$\begin{aligned} C_N(k, \theta_k, \alpha_k; |\omega_0\rangle) &= G_N^{II,k}(\theta_k, \alpha_k; |\omega_0\rangle) |\phi_0\rangle \langle \phi_0| (I_2 \otimes \dots \otimes I_2 \otimes I_2) \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_1\rangle) |\phi_0\rangle \langle \phi_0| (I_2 \otimes \dots \otimes I_2 \otimes \sigma_z) \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_2\rangle) |\phi_0\rangle \langle \phi_0| (I_2 \otimes \dots \otimes \sigma_z \otimes I_2) \\ &\vdots \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_{N-1}\rangle) |\phi_0\rangle \langle \phi_0| (\sigma_z \otimes \dots \otimes \sigma_z \otimes \sigma_z). \end{aligned} \quad (39)$$

By defining the operators,

$$\mathcal{F}_0 = I_2 \otimes \dots \otimes I_2 \otimes I_2 \quad (40)$$

$$\mathcal{F}_1 = I_2 \otimes \dots \otimes I_2 \otimes \sigma_z \quad (41)$$

$$\mathcal{F}_2 = I_2 \otimes \dots \otimes \sigma_z \otimes I_2 \quad (42)$$

$$\vdots$$

$$\mathcal{F}_{N-1} = \sigma_z \otimes \dots \otimes \sigma_z \otimes \sigma_z, \quad (43)$$

(39) is, in a compact form, expressed as

$$\begin{aligned} C_N(k, \theta_k, \alpha_k; |\omega_0\rangle) &= G_N^{II,k}(\theta_k, \alpha_k; |\omega_0\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_0 \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_1\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_1 \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_2\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_2 \\ &\vdots \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_{N-1}\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_{N-1}. \end{aligned} \quad (44)$$

The operators $\mathcal{F}_i$ act as $\mathcal{F}_0|\phi_0\rangle = |\phi_0\rangle$ and $\mathcal{F}_i|\phi_0\rangle = |\phi_0^{(i)}\rangle$ ($i = 1, \dots, N-1$). The term with $\mathcal{F}_0$ extracts the target $|\omega_0\rangle$. In this sense, $\mathcal{F}_i$ are regarded as the so-called filtering operators for the target. By changing the position of $\mathcal{F}_0$, C_N can be a unitary evolution operator for any single target $|\omega_i\rangle$. Although the position of $\mathcal{F}_0$ must be fixed to the assumed target $|\omega_i\rangle$, the positions of the other $\mathcal{F}_i$ ($i = 1, \dots, N-1$) can be any. By using the relation $|\phi_0\rangle \langle \phi_0| = [W_N(-\alpha_k) - I_N e^{-i\alpha_k}]/(1 - e^{-i\alpha_k})$, (44) can be more explicitly written in terms of operators as,

$$\begin{aligned} C_N(k, \theta_k, \alpha_k; |\omega_0\rangle) &= (1 - e^{-i\alpha_k})^{-1} \left\{ G_N^{II,k}(\theta_k, \alpha_k; |\omega_0\rangle) [W_N(-\alpha_k) - I_N e^{-i\alpha_k}] \mathcal{F}_0 \right. \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_1\rangle) [W_N(-\alpha_k) - I_N e^{-i\alpha_k}] \mathcal{F}_1 \\ &+ G_N^{II,k}(\theta_k, \alpha_k; |\omega_2\rangle) [W_N(-\alpha_k) - I_N e^{-i\alpha_k}] \mathcal{F}_2 \\ &\vdots \\ &\left. + G_N^{II,k}(\theta_k, \alpha_k; |\omega_{N-1}\rangle) [W_N(-\alpha_k) - I_N e^{-i\alpha_k}] \mathcal{F}_{N-1} \right\}. \end{aligned} \quad (45)$$

Equation (44) (or (45)) is a unitary search operator in our decomposition scheme. Thus, for any single target $|\omega_i\rangle$ we have $C_N(k, \theta_k, \alpha_k; |\omega_i\rangle)|\phi_0\rangle = G_N^{II,k}(\theta, \alpha_k; |\omega_i\rangle)|\phi_0\rangle = G_N^k(\alpha_k)|\phi_0\rangle$, where only $G_N^{II,k}$ is not unitary as mentioned before. Further, $C_N(k, \theta_k, \alpha_k; |\omega_i\rangle)$ is not identical to the iterative search operator $G_N^k(\alpha_k)$ in general.

In what follows, we examine how C_N defined by (44) or (45) is implemented on a quantum circuit. To make the point clear we illustrate simple examples of $N = 4$.

Example 1: $N = 4$ ($n = 2$), $M = 1$, $\lambda = 1/4$, $|t\rangle = |\omega_0\rangle$

In this case, the optimal k is $k = 1$ for the search with certainty. Hence, $\alpha_1 = \pi$, $\theta_1 = \pi/3$, $g_1(\theta_1) = 1$, $h_1(\theta_1) = -1$ and $v_t = 1$.

From (44), for the assumed $|t\rangle = |\omega_0\rangle$, C_4 is given as

$$\begin{aligned} C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle) &= v_t [|\omega_0\rangle\langle\phi_0|\mathcal{F}_0 + |\omega_1\rangle\langle\phi_0|\mathcal{F}_1 + |\omega_2\rangle\langle\phi_0|\mathcal{F}_2 + |\omega_3\rangle\langle\phi_0|\mathcal{F}_3] \\ &= v_t [|\omega_0\rangle\langle\phi_0|(I_2 \otimes I_2) + |\omega_1\rangle\langle\phi_0|(I_2 \otimes \sigma_z) + |\omega_2\rangle\langle\phi_0|(\sigma_z \otimes I_2) + |\omega_3\rangle\langle\phi_0|(\sigma_z \otimes \sigma_z)] \\ &= v_t (H \otimes H). \end{aligned} \quad (46)$$

Obviously $C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle)|\phi_0\rangle = v_t(H \otimes H)|\phi_0\rangle = v_t|\omega_0\rangle$. In this simple example, it turns out that C_4 leads to the presumably constructed gate $H \otimes H$ directly.

Next, we examine a different choice of the pair of $|\omega_i\rangle$ and $\mathcal{F}_j$ as

$$C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle) = v_t [|\omega_0\rangle\langle\phi_0|\mathcal{F}_0 + |\omega_1\rangle\langle\phi_0|\mathcal{F}_3 + |\omega_2\rangle\langle\phi_0|\mathcal{F}_2 + |\omega_3\rangle\langle\phi_0|\mathcal{F}_1]. \quad (47)$$

This choice leads to the following gate,

$$C_4(k=1, \theta_1, \alpha_1, |\omega_0\rangle) = v_t \left\{ \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \otimes H + \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \otimes R \right\}, \quad (48)$$

where $R = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$. This gate is complicated compared with that of (46), although it gives $C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle)|\phi_0\rangle = v_t|\omega_0\rangle$ properly. Thus, in order to obtain a simple gate the choice of the positions of $\mathcal{F}_i$ ($i = 1, 2, 3$) must be optimal. For other single targets $|\omega_i\rangle$ ($i = 1, 2, 3$) the situation is similar.

Next, we discuss multi-targets cases with two examples of $M = 2$ and 3.

Example 2: $N = 4$ ($n = 2$), $M = 2$, $\lambda = 1/2$, $|t\rangle = |\omega_0\rangle$ and $|\omega_1\rangle$

In this case, the optimal k is $k = 1$ for the search with certainty. Hence, $\alpha_1 = \pi/2$, $\theta_1 = \pi/3$, $g_1(\theta_1) = 1$, $h_1(\theta_1) = -1$ and $v_t = (1 + i)/2$. For the assumed two targets $|\omega_0\rangle$ and $|\omega_1\rangle$, for example, a unitary transformation C_4 is constructed as,

$$\begin{aligned} C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle) &= G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle)|\phi_0\rangle\langle\phi_0|\mathcal{F}_0 \\ &\quad + G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_1\rangle)|\phi_0\rangle\langle\phi_0|\mathcal{F}_1 \\ &\quad + G_4^{II,1}(\theta_1, \alpha_1; |\omega_2\rangle, |\omega_3\rangle)|\phi_0\rangle\langle\phi_0|\mathcal{F}_2 \\ &\quad + G_4^{II,1}(\theta_1, \alpha_1; |\omega_2\rangle, -|\omega_3\rangle)|\phi_0\rangle\langle\phi_0|\mathcal{F}_3, \end{aligned} \quad (49)$$

where

$$G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle)|\phi_0\rangle = [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_0\rangle, |\omega_1\rangle)]|\phi_0\rangle = v_t(|\omega_0\rangle + |\omega_1\rangle) \quad (50)$$

$$G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_1\rangle)|\phi_0\rangle = [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_0\rangle, -|\omega_1\rangle)]|\phi_0\rangle = v_t(|\omega_0\rangle - |\omega_1\rangle) \quad (51)$$

$$G_4^{II,1}(\theta_1, \alpha_1; |\omega_2\rangle, |\omega_3\rangle)|\phi_0\rangle = [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_2\rangle, |\omega_3\rangle)]|\phi_0\rangle = v_t(|\omega_2\rangle + |\omega_3\rangle) \quad (52)$$

$$G_4^{II,1}(\theta_1, \alpha_1; |\omega_2\rangle, -|\omega_3\rangle)|\phi_0\rangle = [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_2\rangle, -|\omega_3\rangle)]|\phi_0\rangle = v_t(|\omega_2\rangle - |\omega_3\rangle). \quad (53)$$

with

$$U_4(-\alpha_1; |\omega_0\rangle, |\omega_1\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_0\rangle\langle\omega_0| + |\omega_1\rangle\langle\omega_1|) \quad (54)$$

$$U_4(-\alpha_1; |\omega_0\rangle, -|\omega_1\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_0\rangle\langle\omega_0| - |\omega_1\rangle\langle\omega_1|) \quad (55)$$

$$U_4(-\alpha_1; |\omega_2\rangle, |\omega_3\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_2\rangle\langle\omega_2| + |\omega_3\rangle\langle\omega_3|) \quad (56)$$

$$U_4(-\alpha_1; |\omega_2\rangle, -|\omega_3\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_2\rangle\langle\omega_2| - |\omega_3\rangle\langle\omega_3|). \quad (57)$$

In deriving (51) and (53), the relation $g_1(\theta_1) + h_1(\theta_1) = 0$ that holds for the search with certainty was effectively used. Eventually, it turns out that the search operator of (49) leads to the presumably constructed unitary gate,

$$C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle) = v_t \sqrt{2} H \otimes I_2. \quad (58)$$

In this case, target state $|T\rangle = \frac{1}{\sqrt{2}}(|\omega_0\rangle + |\omega_1\rangle)$ is not entangled. Therefore, the obtained gate can be presumable. The choice of the positions of $\mathcal{F}_i$ ($i = 1, 2, 3$) in this case is optimal.

Example 3: $N = 4$ ($n = 2$), $M = 3$, $\lambda = 3/4$, $|t\rangle = |\omega_0\rangle, \omega_1\rangle$ and $|\omega_2\rangle$

In this case, the optimal k is $k = 1$ for the search with certainty. Hence, $\alpha_1 = \arccos(1/3)$, $\theta_1 = \pi/3$, $g_1(\theta_1) = 1$, $h_1(\theta_1) = -1$ and $v_t = (i\sqrt{2}-1)/(2i\sqrt{2}+1)$. For the assumed $|\omega_0\rangle$, $|\omega_1\rangle$ and $|\omega_2\rangle$, for example, a unitary transformation C_4 is constructed as

$$\begin{aligned} C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) &= G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_0 \\ &+ G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_1\rangle, |\omega_3\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_1 \\ &+ G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_2\rangle, -|\omega_3\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_2 \\ &+ G_4^{II,1}(\theta_1, \alpha_1; |\omega_1\rangle, -|\omega_2\rangle, |\omega_3\rangle) |\phi_0\rangle \langle \phi_0| \mathcal{F}_3, \end{aligned} \quad (59)$$

where

$$\begin{aligned} G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) |\phi_0\rangle &= [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle)] |\phi_0\rangle \\ &= v_t(|\omega_0\rangle + |\omega_1\rangle + |\omega_2\rangle) \end{aligned} \quad (60)$$

$$\begin{aligned} G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_1\rangle + |\omega_3\rangle) |\phi_0\rangle &= [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_0\rangle, -|\omega_1\rangle, |\omega_3\rangle)] |\phi_0\rangle \\ &= v_t(|\omega_0\rangle - |\omega_1\rangle + |\omega_3\rangle) \end{aligned} \quad (61)$$

$$\begin{aligned} G_4^{II,1}(\theta_1, \alpha_1; |\omega_0\rangle, -|\omega_2\rangle, -|\omega_3\rangle) |\phi_0\rangle &= [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_0\rangle, -|\omega_2\rangle, -|\omega_3\rangle)] |\phi_0\rangle \\ &= v_t(|\omega_0\rangle - |\omega_2\rangle - |\omega_3\rangle) \end{aligned} \quad (62)$$

$$\begin{aligned} G_4^{II,1}(\theta_1, \alpha_1; |\omega_1\rangle, -|\omega_2\rangle, |\omega_3\rangle) |\phi_0\rangle &= [g_1(\theta_1)I_4 + h_1(\theta_1)U_4(-\alpha_1; |\omega_1\rangle, -|\omega_2\rangle, |\omega_3\rangle)] |\phi_0\rangle \\ &= v_t(|\omega_1\rangle - |\omega_2\rangle + |\omega_3\rangle) \end{aligned} \quad (63)$$

with

$$U_4(-\alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_0\rangle\langle\omega_0| + |\omega_1\rangle\langle\omega_1| + |\omega_2\rangle\langle\omega_2|) \quad (64)$$

$$U_4(-\alpha_1; |\omega_0\rangle, -|\omega_1\rangle, |\omega_3\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_0\rangle\langle\omega_0| - |\omega_1\rangle\langle\omega_1| + |\omega_3\rangle\langle\omega_3|) \quad (65)$$

$$U_4(-\alpha_1; |\omega_0\rangle, -|\omega_2\rangle, -|\omega_3\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_0\rangle\langle\omega_0| - |\omega_2\rangle\langle\omega_2| - |\omega_3\rangle\langle\omega_3|) \quad (66)$$

$$U_4(-\alpha_1; |\omega_1\rangle, -|\omega_2\rangle, |\omega_3\rangle) = I_4 - (1 - e^{-i\alpha_1})(|\omega_1\rangle\langle\omega_1| - |\omega_2\rangle\langle\omega_2| + |\omega_3\rangle\langle\omega_3|). \quad (67)$$

It turns out that the search operator of (59) leads to the following unitary gate,

$$C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) = v_t \left\{ I_2 \otimes \frac{1}{2} \begin{bmatrix} 3 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \otimes \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 3 \end{bmatrix} \right\}. \quad (68)$$

In this case, target state $|T\rangle = \frac{1}{\sqrt{3}}(|\omega_0\rangle + |\omega_1\rangle + |\omega_2\rangle)$ is entangled. Therefore, the obtained gate is not presumable. Other choices of the positions of $\mathcal{F}_i$ ($i = 1, \dots, 3$) do not improve this situation.

It should be stressed that the transformations C_4 of these examples are not all the same as the corresponding G_4 of the iterative search, although both C_4 and G_4 give the same search state $|\phi_1\rangle$, i.e., $C_4|\phi_0\rangle = G_4|\phi_0\rangle = |\phi_1\rangle$. The gates of C_4 are simpler than those of G_4 . We illustrate this in Appendix B by comparing matrix C_4 of Example 3 and matrix G_4 .

Before ending this section, we consider a parallel processing system implied by the reduced form of (26). It represents that the final search state $|\phi_k\rangle$ is given as a superposition of $|\phi_0\rangle$ and $|\phi_U\rangle \equiv U_N(-\alpha)|\phi_0\rangle$. This may imply a parallel processing scheme with two inputs ($|\phi_0\rangle$ and $|\phi_U\rangle$) and two outputs ($|\phi_k\rangle$ and an ancillary state $|\chi\rangle$). In Appendix C we present an analysis of this scheme. We show that this two-channel processing can be decoupled into the single processing of Fig. 2 that we examined in the present section and an ancillary single processing.

IV. SUMMARY AND DISCUSSION

We have derived an additive decomposition scheme of an iterative phase-matching search algorithm of the Grover type, in which a k -iterative search process is, in the computational space, expressed as a linear combination of k one-time searches followed by overall phase-rotations. The phase rotation parameter θ is preliminarily determined by the fraction λ of the targets and a matching phase α . We emphasize that in the decomposition, the number of oracle operations remains the same. The decomposed form can be rewritten such that the final state is simply expressed as a superposition of the initial database state and a one-time searched state, where superposition coefficients consist of θ alone as shown in (23). We further showed that the decomposed form can be reduced to the form where the final state is expressed in terms of only a *single oracle operator* (without any diffusion operator; see (26)). The decomposition holds for any k , α , λ and the number of qubit-registers n , as long as θ is determined by (10). Although it yields the norm of the final state correctly, the reduced operator $G_N^{I,k}(\alpha)$ itself in the decomposed form of (23) is not unitary in general. Thus $G_N^{I,k}(\alpha)$ cannot directly be implemented as quantum mechanical evolution by unitary gates. Therefore, by utilizing the advantage of $G_N^{II,k}(\alpha)$ of (26) we proposed a unitary transformation that directly transforms the initial database state to the final state. To determine the unitary transformation we only need the information on the one-time oracle operation on the initial state[21].

For the exact search [7] with the desired success probability $P_k(\lambda) = 1$ for $0 < \lambda \leq 1$, the construction of the unitary transformation can be much simplified because the components of the final state vector have nonzero values only for the components corresponding to the target basis states. In their matrix representations, the unitary transformation is much simpler than the original k iterative search operation. As an example we illustrated this situation explicitly for the case of $n = 3$ ($N = 8$), $k = 2$ and one target. An effective reduction of the computational load is important in particular in the situation with a small λ (namely, a small number of targets), in which the final state of the exact search algorithm becomes very simple.

Let us add that for the search problem where λ is not given preliminarily, the multi-phase matching (MPM) method [16–19] is useful. The MPM yields the success probability $P_k(\lambda)$ that is almost constant and unity over a wide range of λ , i.e., $P(\lambda) \simeq 1$ for $0 < \lambda \leq 1$. This MPM method enables searches with certainty with no information of λ . Instead, in MPM method the number of iterations k is fixed preliminarily for an iterative search with an arbitrary λ , where k is determined in finding the matched multi-phases. Therefore, for a larger range of λ s the number of iterations k of MPM is much larger than that of the exact search with $P_k(\lambda) = 1$ reviewed in Sec. II. It would be meaningful to examine whether or not a similar scheme of reducing the computational load of the MPM method effectively is possible.

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Appendix A: An illustration of the additive decomposition of the iterative Grover search in computational space

We give an illustration of the additive decomposition scheme of the iterative Grover search. As an example, we consider the case of $n = 3$ ($N = 8$) and a target $|t_0\rangle = |000\rangle$. In this case $\lambda = 1/8$. Hence, the optimal number of searches for the exact search is $k = 2$ (see (5)). In the computational space, $|\phi_0\rangle = \frac{1}{\sqrt{8}}(1, 1, 1, 1, 1, 1, 1, 1)^T$ and $|\omega_0\rangle = |000\rangle = (1, 0, 0, 0, 0, 0, 0, 0)^T$, where T indicates *transposed*. In the eight-dimensional computation space, the search operator $G_8(\alpha_2)$ is represented as

$$G_8(\alpha_2) = W_8(-\alpha_2)U_8(\alpha_2)$$

$$= \frac{1}{8} \begin{pmatrix} A^* + 7 & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A \\ A^* - 1 & 1 + 7A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A \\ A^* - 1 & 1 - A & 1 + 7A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A \\ A^* - 1 & 1 - A & 1 - A & 1 + 7A & 1 - A & 1 - A & 1 - A & 1 - A \\ A^* - 1 & 1 - A & 1 - A & 1 - A & 1 + 7A & 1 - A & 1 - A & 1 - A \\ A^* - 1 & 1 - A & 1 - A & 1 - A & 1 - A & 1 + 7A & 1 - A & 1 - A \\ A^* - 1 & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 + 7A & 1 - A \\ A^* - 1 & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 - A & 1 + 7A \end{pmatrix}, \quad (\text{A.1})$$

where $A = e^{-i\alpha_2}$. With this $G_8(\alpha_2)$ of (A.1), the final state $|\phi_2\rangle = G_8^2(\alpha_2)|\phi_0\rangle$ is given as

$$|\phi_2\rangle = \frac{\sqrt{2}}{64} \begin{pmatrix} -(3 \cos \alpha_2 + 14) \cos \alpha_2 + 33 + i4(\cos \alpha_2 + 7) \sin \alpha_2 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \\ \cos^2 \alpha_2 + 10 \cos \alpha_2 + 5 \end{pmatrix}. \quad (\text{A.2})$$

The matching phase α_2 for the exact search is given as (see (4)),

$$\alpha_2 = \arccos[1 - 8(1 - \cos(\pi/5))] = \arccos(-5 + 2\sqrt{5}). \quad (\text{A.3})$$

With this α_2 , (A.2) turns out to be

$$|\phi_2\rangle = \frac{1}{\sqrt{8}} \left(2(\sqrt{5} - 1) + i\sqrt{5\sqrt{5} - 11} (\sqrt{5} + 1), 0, 0, 0, 0, 0, 0, 0 \right)^T. \quad (\text{A.4})$$

The modulus of the first component of (A.4) is unity, namely $\left| \frac{1}{\sqrt{8}} [2(\sqrt{5} - 1) + i\sqrt{5\sqrt{5} - 11} (\sqrt{5} + 1)] \right| = 1$. Thus, an exact search is completed.

Next, we consider the decomposed form, (21),

$$|\phi_2\rangle = G_8^2(\alpha_2)|\phi_0\rangle = [e^{i\theta} G_8(\alpha_2) + e^{-i\theta} G_8(\alpha_2) + e^{i\pi} I_8] |\phi_0\rangle. \quad (\text{A.5})$$

The first and second terms of the r.h.s. of (A.5) are

$$e^{\pm i\theta_2} G_8(\alpha_2) |\phi_0\rangle = e^{\pm i\theta_2} \frac{\sqrt{2}}{32} \begin{pmatrix} 14 + e^{i\alpha_2} - 7e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \\ 6 + e^{i\alpha_2} + e^{-i\alpha_2} \end{pmatrix}. \quad (\text{A.6})$$

The third term in the r.h.s. of (A.5) is $e^{i\pi} I_8 |\phi_0\rangle = -\frac{1}{\sqrt{8}}(1, 1, 1, 1, 1, 1, 1, 1)^T$. Accordingly, (A.5) is represented as

$$\begin{aligned} |\phi_2\rangle &= [e^{i\theta_2} G_8(\alpha_2) + e^{-i\theta_2} G_8(\alpha_2) + e^{i\pi} I_8] |\phi_0\rangle \\ &= \frac{\sqrt{2}}{8} \begin{pmatrix} \cos \theta_2 (7 - 3 \cos \alpha_2 + i 4 \sin \alpha_2) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \\ \cos \theta_2 (\cos \alpha_2 + 3) - 2 \end{pmatrix}. \end{aligned} \quad (\text{A.7})$$

From (10), $\cos \theta_2 = (7 + \cos \alpha_2)/8$. By using this relation, (A.7) is reduced to (A.2). Furthermore, with the overall rotation phase $\theta_2 = \pi/(2k+1) = \pi/5$ and α_2 of (A.3), (A.7) is reduced to (A.4). This illustration verifies that the additive decomposition formula of the state vector $|\phi_k\rangle$ of (21) (or (23) or (26)) is correct as an identity.

Appendix B: Comparison between the matrix representations of C_4 of Eq. (68) and G_4

The complexity of C_4 of Eq. (68) of Example 3 and the corresponding G_4 of the iterative search is compared in their matrix representations. The matrix of C_4 is

$$C_4(k=1, \theta_1, \alpha_1; |\omega_0\rangle, |\omega_1\rangle, |\omega_2\rangle) = v_t \begin{pmatrix} 3/2 & 1/2 & 1/2 & -1/2 \\ 1/2 & 1/2 & -1/2 & 3/2 \\ -1/2 & 1/2 & 3/2 & 1/2 \\ 1/2 & -3/2 & 1/2 & 1/2 \end{pmatrix}, \quad (\text{B.1})$$

where $v_t = (i\sqrt{2} - 1)/(2i\sqrt{2} + 1)$. On the other hand, the matrix of G_4 is more complex as,

$$G_4(\alpha_1) = v_t \begin{pmatrix} \frac{11\sqrt{2}i+1}{6\sqrt{2}i-6} & \sqrt{2}i/3+1/6 & \sqrt{2}i/3+1/6 & 1/2 \\ \sqrt{2}i/3+1/6 & \frac{11\sqrt{2}i+1}{6\sqrt{2}i-6} & \sqrt{2}i/3+1/6 & 1/2 \\ \sqrt{2}i/3+1/6 & \sqrt{2}i/3+1/6 & \frac{11\sqrt{2}i+1}{6\sqrt{2}i-6} & 1/2 \\ \sqrt{2}i/3+1/6 & \sqrt{2}i/3+1/6 & \sqrt{2}i/3+1/6 & \frac{\sqrt{2}i+5}{2\sqrt{2}i-2} \end{pmatrix}. \quad (\text{B.2})$$

Note that $C_4|\phi_0\rangle = G_4|\phi_0\rangle = |\phi_1\rangle$.

Appendix C: A parallel processing scheme suggested by the reduced form of (26)

The reduced form of (26) might imply the parallel processing scheme shown in Fig. 2. Mathematically it is understood that the input state is the tensor product state of $|\phi_0\rangle$ and $|\phi_U\rangle$, where each state is N -dimensional. The input state is thus N^2 -dimensional. The output state is expressed as a tensor product state of the final-search state $|\phi_k\rangle$ and an ancillary N -dimensional state $|\chi\rangle$, which is needed for consistency of dimensions between the input and output states. The state $|\chi\rangle$ can be taken appropriately in constructing unitary transformation. In the scheme it is assumed that the superposition coefficients $g_k(\theta)$ and $h_k(\theta)$ are incorporated in the transformation D_N . Hence the parallel processing scheme shown in Fig. 2 can be mathematically expressed as

$$|\phi_2\rangle \otimes |\chi\rangle = D_N(k, \theta_k, \alpha_k) (|\phi_0\rangle \otimes |\phi_U\rangle). \quad (\text{C.1})$$

We can write the unitary transformation D_N as

$$D_N(k, \theta_k, \alpha_k) = \sum_{j=0}^{N^2-1} |\Psi_2^{(j)}\rangle \langle \Psi_0^{(j)}|, \quad (\text{C.2})$$

where $|\Psi_0^{(j)}\rangle$ and $|\Psi_2^{(j)}\rangle$ are respectively N^2 -dimensional orthonormal sets, namely $\langle \Psi_0^{(i)} | \Psi_0^{(j)} \rangle = \delta_{ij}$ and $\langle \Psi_2^{(i)} | \Psi_2^{(j)} \rangle = \delta_{ij}$. Thus D_N is obviously unitary because the completeness holds for each set $|\Psi_2^{(j)}\rangle (j = 0, \dots, N^2 - 1)$ and $|\Psi_0^{(j)}\rangle (j = 0, \dots, N^2 - 1)$. The $|\Psi_0^{(j)}\rangle$ and $|\Psi_2^{(j)}\rangle$ can respectively be tensor product states such as

$$|\Psi_0^{(j)}\rangle = |\phi_0^{(p)}\rangle \otimes |\phi_U^{(q)}\rangle, \quad (\text{C.3})$$

$$|\Psi_2^{(j)}\rangle = |\phi_2^{(p)}\rangle \otimes |\chi^{(q)}\rangle, \quad (\text{C.4})$$

where $(p, q) = 0, \dots, N - 1$ and $|\phi_0^{(0)}\rangle \equiv |\phi_0\rangle$, $|\phi_2^{(0)}\rangle \equiv |\phi_2\rangle$, $|\phi_U^{(0)}\rangle \equiv |\phi_U\rangle$ and $|\chi^{(0)}\rangle \equiv |\chi\rangle$. Further, $|\phi_2^{(p)}\rangle$, $|\phi_U^{(q)}\rangle$ and $|\chi^{(q)}\rangle$ are respectively taken to be orthonormal to each other, i.e., $\langle \phi_0^{(p)} | \phi_0^{(q)} \rangle = \delta_{pq}$, $\langle \phi_2^{(p)} | \phi_2^{(q)} \rangle = \delta_{pq}$, $\langle \phi_U^{(p)} | \phi_U^{(q)} \rangle = \delta_{pq}$ and $\langle \chi^{(p)} | \chi^{(q)} \rangle = \delta_{pq}$. By these definitions, the orthonormality $\langle \Psi_0^{(i)} | \Psi_0^{(j)} \rangle = \delta_{ij}$ and $\langle \Psi_2^{(i)} | \Psi_2^{(j)} \rangle = \delta_{ij}$ are guaranteed.

FIG. 2: (Colour online) Parallel processing scheme implied by the reduced form of (26), i.e., $|\phi_k\rangle = [g_k(\theta)I_N + h_k(\theta)U_N(-\alpha)]|\phi_0\rangle \equiv g_k(\theta)|\phi_0\rangle + h_k(\theta)|\phi_U\rangle$, where $|\phi_U\rangle \equiv U_N(-\alpha)|\phi_0\rangle$. The ancillary state $|\chi\rangle$ is needed for consistency of the dimensions between the input and output states, which we can take appropriately in constructing a unitary transformation $D_N(k, \theta_k, \alpha_k)$.

In the following we discuss explicitly the structure of the unitary transformation D_N of (C.2). For simplicity we examine D_N for the case of $N = 2$ ($n = 1$). The generalization to any N is straightforward. The D_N can be written as,

$$\begin{aligned} D_N(k, \theta_k, \alpha_k) &= \sum_{j=0}^{2^2-1} |\Psi_2^{(j)}\rangle \langle \Psi_0^{(j)}| \\ &= (|\phi_2^{(0)}\rangle \otimes |\chi^{(0)}\rangle) (\langle \phi_0^{(0)}| \otimes \langle \phi_U^{(0)}|) \\ &\quad + (|\phi_2^{(0)}\rangle \otimes |\chi^{(1)}\rangle) (\langle \phi_0^{(0)}| \otimes \langle \phi_U^{(1)}|) \\ &\quad + (|\phi_2^{(1)}\rangle \otimes |\chi^{(0)}\rangle) (\langle \phi_0^{(1)}| \otimes \langle \phi_U^{(0)}|) \\ &\quad + (|\phi_2^{(1)}\rangle \otimes |\chi^{(1)}\rangle) (\langle \phi_0^{(1)}| \otimes \langle \phi_U^{(1)}|). \end{aligned} \quad (\text{C.5})$$

Equation (C.5) is manipulated as

$$\begin{aligned} D_N(k, \theta_k, \alpha_k) &= |\phi_2^{(0)}\rangle \langle \phi_0^{(0)}| \otimes |\chi^{(0)}\rangle \langle \phi_U^{(0)}| \\ &\quad + |\phi_2^{(0)}\rangle \langle \phi_0^{(0)}| \otimes |\chi^{(1)}\rangle \langle \phi_U^{(1)}| \\ &\quad + |\phi_2^{(1)}\rangle \langle \phi_0^{(1)}| \otimes |\chi^{(0)}\rangle \langle \phi_U^{(0)}| \\ &\quad + |\phi_2^{(1)}\rangle \langle \phi_0^{(1)}| \otimes |\chi^{(1)}\rangle \langle \phi_U^{(1)}|. \end{aligned} \quad (\text{C.6})$$

$$\begin{aligned}
&= \left(|\phi_2^{(0)}\rangle \langle \phi_0^{(0)}| + |\phi_2^{(1)}\rangle \langle \phi_0^{(1)}| \right) \\
&\otimes \left(|\chi^{(0)}\rangle \langle \phi_U^{(0)}| + |\chi^{(1)}\rangle \langle \phi_U^{(1)}| \right).
\end{aligned} \tag{C.7}$$

The final form of (C.7) implies that the states $|\phi_0\rangle$ and $|\phi_U\rangle$ in the input channel are separately transformed to the output states $|\phi_2\rangle$ and $|\chi\rangle$, namely

$$\begin{aligned}
&D_N(k, \theta_k, \alpha_k) \left(|\phi_0^{(0)}\rangle \otimes |\phi_U^{(0)}\rangle \right) \\
&= \left[\left(|\phi_2^{(0)}\rangle \langle \phi_0^{(0)}| + |\phi_2^{(1)}\rangle \langle \phi_0^{(1)}| \right) \right. \\
&\quad \left. \otimes \left(|\chi^{(0)}\rangle \langle \phi_U^{(0)}| + |\chi^{(1)}\rangle \langle \phi_U^{(1)}| \right) \right] \left(|\phi_0^{(0)}\rangle \otimes |\phi_U^{(0)}\rangle \right) \\
&= |\phi_2^{(0)}\rangle \otimes |\chi^{(0)}\rangle.
\end{aligned} \tag{C.8}$$

This means that the two-channel parallel-processing scheme suggested by the reduced form of (26) is equivalent to the decoupled two one-channel schemes for the inputs $|\phi_0\rangle$ and $|\phi_U\rangle$. This situation of the decoupling of two channels is the same even if the channels 1 and 2 in the initial state are exchanged.

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