Dynamical analysis of Grover's search algorithm in arbitrarily high-dimensional search spaces

Wenliang Jin*
College of Information Engineering, Yangzhou University, Yangzhou, Jiangsu 225127, People's Republic of China
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We discuss at length the dynamical behavior of Grover's search algorithm for which all the Walsh-Hadamard transformations contained in this algorithm are exposed to their respective random perturbations inducing the augmentation of the dimension of the search space. We give the concise and general mathematical formulations for approximately characterizing the maximum success probabilities of finding a unique desired state in a large unsorted database and their corresponding numbers of Grover iterations, which are applicable to the search spaces of arbitrary dimension and are used to answer a salient open problem posed by Grover [L. K. Grover, Phys. Rev. Lett. **80**, 4329 (1998)].

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I. INTRODUCTION

The quantum search algorithm [1] discovered by Grover allows one to find a single desired state in a large unsorted database of size N using merely a number of queries in $\Theta(\sqrt{N})$, compared to the classical $\Theta(N)$, thus providing a quadratic speedup; and it was shown to be optimal in the sense that it is as efficient as theoretically possible according to Refs. [2–4]. It is well-known that quantum systems are inevitably subject to some unfavorable ingredients such as decoherence, perturbation, noise, imperfection, error, and so on [5]. The decoherence effect caused by the interaction between a quantum computer and its environment has been thought of as one of the most serious difficulties in implementation of quantum computation [5–10]. To prevent loss of information of a quantum computer due to the occurrence of decoherence or perturbation, the concept of quantum error correction was introduced [11–14]. Undoubtedly, whether in theoretical or practical contexts, it is of significance to further investigate the evolution of a quantum system subjected to various perturbations, arising from either external environmental interactions or internal effects. In [15], Grover showed that his algorithm can be implemented by replacing the Walsh-Hadamard transformation on n qubits $W = H^{\otimes n}$ by (*almost*) any unitary transformation U, where H is single-qubit Hadamard gate operation and $\otimes$ stands for tensor product. Meanwhile, he noticed that such framework demands that U and U^{-1} stay the same at all time steps, where the superscript $^{-1}$ refers to the inverse of an operator. Inspired by this limitation, Grover formulated his own opinion on the problem addressed: "*What happens if there are small perturbations in these? It seems plausible that these will not create much of an impact if they are small and average out to zero; however, that is something still to be proved*". This formulation can be regarded as tantamount to an interesting attempt to consider the case for search spaces of any finite dimension in the case that those small perturbations are not fixed but average out to zero. Thereafter, the problem of the influence of noise or perturbation on the behavior of Grover's search algorithm was extensively explored [16–20].

In order to corroborate Grover's verdict, here, for clarity of presentation, we will assume that we transform, on applying W, the initial zero state $|0\rangle \equiv |00\cdots0\rangle \equiv |0\rangle^{\otimes n}$ into

$$|\gamma_0\rangle = \frac{1}{\sqrt{N}}\sum_{x=0}^{N-1}|x\rangle = \cos t\,|\alpha\rangle + \sin t\,|\beta\rangle\,, \tag{1}$$

an initial unbiased uniform superposition of all $N = 2^n$ computational basis states. Here $|\beta\rangle$ is some item we are looking for in an unsorted database of N entries, the normalized basis vectors $|\alpha\rangle$ and the angle t between $|\gamma_0\rangle$ and $|\alpha\rangle$ are given by $|\alpha\rangle = \sum_{x\neq\beta}|x\rangle/\sqrt{N-1}$ and $t = \arcsin\left(\sqrt{1/N}\right)$, respectively, where $\arcsin(\bullet)$ is defined as $-\pi/2 \leq \arcsin(\bullet) \leq \pi/2$. Then, after j sequential applications of the Grover iteration $G = -WI_0W^{-1}I_\beta$, in which $I_\beta = I - 2|\beta\rangle\langle\beta|$ and $I_0 = I - 2|0\rangle\langle 0|$, I being the identity operator, to the initial superposition $|\gamma_0\rangle = W|0\rangle$, we obtain a resulting state:

$$|\psi_j\rangle = \overbrace{\left(-WI_0W^{-1}I_\beta\right)\cdots\left(-WI_0W^{-1}I_\beta\right)}^{j}W|0\rangle\,. \tag{2}$$

Subsequently, we introduce a sequence of $2j+1$ perturbations $\Delta W_0, \Delta W_1, \Delta W_2, \cdots, \Delta W_{2j-1}, \Delta W_{2j}$ sequentially imposed on the Walsh-Hadamard transformations W on the right-hand side of Eq. (2) from right to left such that $|\psi_j\rangle$ turns into another quantum state

$$|\psi_j'\rangle = G_j\cdots G_1|\mu_0\rangle\,, \tag{3}$$

to allow the augmentation of the dimension of the search space, where $|\mu_0\rangle = W_0|0\rangle$ and $G_k = -W_{2k}I_0W_{2k-1}^{-1}I_\beta$, $k = 1,\cdots,j$, where $W_0 = W + \Delta W_0$, $W_{2k-1} = W + \Delta W_{2k-1}$ and $W_{2k} = W + \Delta W_{2k}$ are all unitary operators. Now for each k, the Grover iteration $G_k = -W_{2k}I_0W_{2k-1}^{-1}I_\beta$ reads

$$G_k = -\left(W_{2k}W_{2k-1}^{-1} - 2|\mu_{2k}\rangle\langle\mu_{2k-1}|\right)\left(I - 2|\beta\rangle\langle\beta|\right) \tag{4}$$

or

$$G_k = -\left(W_{2k}W_{2k-1}^{-1}\right)\left(I - 2|\mu_{2k-1}\rangle\langle\mu_{2k-1}|\right)\left(I - 2|\beta\rangle\langle\beta|\right) \tag{5}$$

*wenliang20021@aliyun.com; wenliang20021@yahoo.cn

with $\left|\mu_{2k-1}\right\rangle = W_{2k-1}\left|0\right\rangle$, $\left|\mu_{2k}\right\rangle = W_{2k}\left|0\right\rangle = \left(W_{2k}W_{2k-1}^{-1}\right)\left|\mu_{2k-1}\right\rangle$.

In the present paper, by considering search space constructions as *dynamic* constructions in which all of the state vectors $\left|\mu_0\right\rangle, \left|\mu_1\right\rangle, \left|\mu_2\right\rangle, \cdots, \left|\mu_{2j-1}\right\rangle, \left|\mu_{2j}\right\rangle$ are allowed to deviate from the Grover plane L spanned by $|\alpha\rangle$ and $|\beta\rangle$ freely, we deduce the approximations of the maximum success probabilities of finding the desired state $|\beta\rangle$ in a large database that consists of N unsorted objects and their corresponding numbers of Grover iterations for search spaces of any finite dimension. Our result shows that even when the perturbations $\Delta W_1, \Delta W_2, \cdots, \Delta W_{2j-1}, \Delta W_{2j}$ are not small but meet certain conditions with the vanishing of the perturbation ΔW_0, the effectiveness of Grover's search algorithm can still be guaranteed, independent of whether the dimension of the search space increases during the evolution of the algorithm, whereby we substantiate the foregoing prediction put forward by Grover [15] and further expand its scope of applicability.

II. FOUR-DIMENSIONAL ORTHOGONAL MATRIX REPRESENTATION

Naturally, $\left|\mu_0\right\rangle, \left|\mu_1\right\rangle, \left|\mu_2\right\rangle, \cdots, \left|\mu_{2j-1}\right\rangle, \left|\mu_{2j}\right\rangle$ have to deviate from L due to the presence of corresponding perturbations in general. These superposed states correspond to their respective sets of real numbers $T_l = \{c_{(l,0)}, c_{(l,1)}, \ldots, c_{(l,N-1)}\}$, $l = 0, 1, 2, \cdots, 2j-1, 2j$, with the normalization conditions $\sum_{x=0}^{N-1}\left|c_{(l,x)}\right|^2 = 1$, and may be written as

$$\left|\mu_l\right\rangle = \sum_{x=0}^{N-1} c_{(l,x)}\left|x\right\rangle = \cos\xi_l\left|\alpha_l\right\rangle + \sin\xi_l\left|\beta\right\rangle, \qquad (6)$$

where, for each state vector $\left|\mu_l\right\rangle$, the normalized superposition of the undesired states $\left|\alpha_l\right\rangle$ is given by

$$\left|\alpha_l\right\rangle = \frac{1}{\sqrt{\sum_{x\neq\beta}\left|c_{(l,x)}\right|^2}}\sum_{x\neq\beta} c_{(l,x)}\left|x\right\rangle,$$

and the angle $\xi_l = \arcsin\left(c_{(l,x=\beta)}\right)$ satisfies

$$0 < \xi_l < t. \qquad (7)$$

Here and in what follows, for discussional convenience we shall assume

$$\xi_l \le \xi_0 \qquad \text{for } 1 \le l \le 2j. \qquad (8)$$

For the moment let

$$\left|\mu_1\right\rangle = \cdots = \left|\mu_{2j-1}\right\rangle \qquad (9)$$

$$\text{and} \qquad \left|\mu_2\right\rangle = \cdots = \left|\mu_{2j}\right\rangle. \qquad (10)$$

When the two state vectors $\left|\mu_1\right\rangle$ and $\left|\mu_2\right\rangle$ are linearly independent and lie outside the two-dimensional real subspace L_0 spanned by $\left|\alpha_0\right\rangle$ and $|\beta\rangle$, we can get the following unit vectors

$$\left|S_{l'}\right\rangle = \frac{1}{\sqrt{1-\left|\left\langle\alpha_0|\mu_{l'}\right\rangle\right|^2-\left|\left\langle\beta|\mu_{l'}\right\rangle\right|^2}} \times\left(\left|\mu_{l'}\right\rangle - \left\langle\alpha_0|\mu_{l'}\right\rangle\left|\alpha_0\right\rangle - \left\langle\beta|\mu_{l'}\right\rangle\left|\beta\right\rangle\right), \quad l' = 1, 2, \qquad (11)$$

which are both perpendicular to L_0 by means of the Gram-Schmidt orthogonalization process. Noting that every $\left|S_{l'}\right\rangle$ is a superposition of the undesired states we immediately arrive at

$$\left|S_1^{\perp}\right\rangle = \frac{1}{\sqrt{1-\left|\left\langle S_1|S_2\right\rangle\right|^2}}\left(\left|S_2\right\rangle - \left\langle S_1|S_2\right\rangle\left|S_1\right\rangle\right) \qquad (12)$$

that is orthogonal to $\left|S_1\right\rangle$ and lies in the plane of $\left|S_1\right\rangle$ and $\left|S_2\right\rangle$. This equality leads to the relationship

$$\left|S_2\right\rangle = \cos\omega_2'\left|S_1\right\rangle + \sin\omega_2'\left|S_1^{\perp}\right\rangle \qquad (13)$$

with

$$0 \le \omega_2' = \arccos\left(\left\langle S_1|S_2\right\rangle\right) < \pi/2, \qquad (14)$$

where $\arccos(\bullet)$ is defined as $0 \le \arccos(\bullet) \le \pi$. This relation remains valid for $\omega_2' = 0$, namely $\left|S_2\right\rangle = \left|S_1\right\rangle$, a situation that arises when the state vectors $\left|\mu_1\right\rangle, \left|\mu_2\right\rangle \notin L_0$ constructed as above are actually linearly dependent. $\left|\mu_1\right\rangle$ and $\left|\mu_2\right\rangle$ can then be parametrized by the respective angles ϕ_1, ω_1 and ϕ_2, ω_2, ω_2' according to

$$\left|\mu_1\right\rangle = \sin\omega_1\cos\phi_1\left|\alpha_0\right\rangle + \sin\omega_1\sin\phi_1\left|\beta\right\rangle + \cos\omega_1\left|S_1\right\rangle \qquad (15)$$

and

$$\left|\mu_2\right\rangle = \sin\omega_2\cos\phi_2\left|\alpha_0\right\rangle + \sin\omega_2\sin\phi_2\left|\beta\right\rangle + \cos\omega_2\left|S_2\right\rangle \qquad (16)$$

$$= \sin\omega_2\cos\phi_2\left|\alpha_0\right\rangle + \sin\omega_2\sin\phi_2\left|\beta\right\rangle + \cos\omega_2\cos\omega_2'\left|S_1\right\rangle + \cos\omega_2\sin\omega_2'\left|S_1^{\perp}\right\rangle \qquad (17)$$

with $\phi_1, \phi_2 \in (0, \xi_0]$ and $\omega_1, \omega_2 \in (0, \pi)$.

To facilitate computation, we define the orthonormal basis vectors of quadruples $\left|\alpha_0\right\rangle \equiv (1,0,0,0)^T$, $|\beta\rangle \equiv (0,1,0,0)^T$, $\left|S_1\right\rangle \equiv (0,0,1,0)^T$, $\left|S_1^{\perp}\right\rangle \equiv (0,0,0,1)^T$, where the superscript ^{T} denotes the transpose of a vector.

According to Eq. (4), the matrix representation of

$$G_1 = -\left(W_2W_1^{-1} - 2\left|\mu_2\right\rangle\left\langle\mu_1\right|\right)\left(I - 2\left|\beta\right\rangle\left\langle\beta\right|\right) \qquad (18)$$

can be calculated explicitly if the matrix representation of $W_2W_1^{-1}$ that satisfies

$$\left(W_2W_1^{-1}\right)\left|\mu_1\right\rangle = \left|\mu_2\right\rangle \qquad (19)$$

is determined with respect to the same ordered orthonormal basis $\{\left|\alpha_0\right\rangle, |\beta\rangle, \left|S_1\right\rangle, \left|S_1^{\perp}\right\rangle\}$, which we denote by E_1. The latter may be found as follows. We first choose arbitrarily an ordered orthonormal basis $E_2 = \{\left|\mu_1\right\rangle, \left|\mu_1^{\perp}\right\rangle, \left|e_1\right\rangle, \left|e_2\right\rangle\}$ in the real four-dimensional subspace spanned by E_1, so that the matrix representation of $W_2W_1^{-1}$ is of the form

$$M_2 = \begin{pmatrix} \cos\vartheta_1 & -\sin\vartheta_1 & 0 & 0 \\ \sin\vartheta_1 & \cos\vartheta_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad (20)$$

where ϑ_1 is the angle between $|\mu_1\rangle$ and $|\mu_2\rangle$, i.e.

$$\cos\vartheta_1 = \langle \mu_1 \mid \mu_2\rangle = \sin\omega_1 \sin\omega_2 \cos(\phi_2 - \phi_1) + \cos\omega_1 \cos\omega_2 \cos\omega_2', \quad (21)$$

$$\left|\mu_1^{\perp}\right\rangle = \frac{|\mu_2\rangle - \cos\vartheta_1 |\mu_1\rangle}{\sin\vartheta_1}, \quad (22)$$

here, we do not specify $|e_1\rangle$ and $|e_2\rangle$, but only mention their existence, due to the freedom of choice of these two basis vectors. Then the transition matrix for the basis transformation from E_1 to E_2 will be

$$T_1 = \begin{pmatrix} d_{11} & d_{12} & * & * \\ d_{21} & d_{22} & * & * \\ d_{31} & d_{32} & * & * \\ d_{41} & d_{42} & * & * \end{pmatrix}, \quad (23)$$

where $d_{11} = \sin\omega_1 \cos\phi_1$, $d_{21} = \sin\omega_1 \sin\phi_1$, $d_{31} = \cos\omega_1$, $d_{41} = 0$,

$$\begin{aligned} d_{12} &= \frac{\sin\omega_2 \cos\phi_2 - \cos\vartheta_1 \sin\omega_1 \cos\phi_1}{\sin\vartheta_1}, \\ d_{22} &= \frac{\sin\omega_2 \sin\phi_2 - \cos\vartheta_1 \sin\omega_1 \sin\phi_1}{\sin\vartheta_1}, \\ d_{32} &= \frac{\cos\omega_2 \cos\omega_2' - \cos\vartheta_1 \cos\omega_1}{\sin\vartheta_1}, \\ d_{42} &= \frac{\cos\omega_2 \sin\omega_2'}{\sin\vartheta_1}, \end{aligned}$$

and the $*$'s denote entries which we do not specify further. Using the orthogonality of T_1, in the first basis E_1 the matrix representation of $W_2 W_1^{-1}$ is given by

$$M_1 = T_1 M_2 T_1^{-1} = \begin{pmatrix} g_{11} & g_{12} & g_{13} & g_{14} \\ g_{21} & g_{22} & g_{23} & g_{24} \\ g_{31} & g_{32} & g_{33} & g_{34} \\ g_{41} & g_{42} & g_{43} & g_{44} \end{pmatrix},$$

where

$$\begin{aligned} g_{11} &= (\cos\vartheta_1 - 1)\left(d_{11}^2 + d_{12}^2\right) + 1, \\ g_{12} &= (\cos\vartheta_1 - 1)(d_{11}d_{21} + d_{12}d_{22}) + \sin\vartheta_1 (d_{21}d_{12} - d_{11}d_{22}), \\ g_{13} &= (\cos\vartheta_1 - 1)(d_{11}d_{31} + d_{12}d_{32}) + \sin\vartheta_1 (d_{31}d_{12} - d_{11}d_{32}), \\ g_{14} &= (\cos\vartheta_1 - 1) d_{12}d_{42} - \sin\vartheta_1 d_{11}d_{42}, \\ g_{21} &= (\cos\vartheta_1 - 1)(d_{11}d_{21} + d_{12}d_{22}) + \sin\vartheta_1 (d_{11}d_{22} - d_{21}d_{12}), \\ g_{22} &= (\cos\vartheta_1 - 1)\left(d_{21}^2 + d_{22}^2\right) + 1, \\ g_{23} &= (\cos\vartheta_1 - 1)(d_{21}d_{31} + d_{22}d_{32}) + \sin\vartheta_1 (d_{31}d_{22} - d_{21}d_{32}), \\ g_{24} &= (\cos\vartheta_1 - 1) d_{22}d_{42} - \sin\vartheta_1 d_{21}d_{42}, \\ g_{31} &= (\cos\vartheta_1 - 1)(d_{11}d_{31} + d_{12}d_{32}) + \sin\vartheta_1 (d_{11}d_{32} - d_{31}d_{12}), \\ g_{32} &= (\cos\vartheta_1 - 1)(d_{21}d_{31} + d_{22}d_{32}) + \sin\vartheta_1 (d_{21}d_{32} - d_{31}d_{22}), \\ g_{33} &= (\cos\vartheta_1 - 1)\left(d_{31}^2 + d_{32}^2\right) + 1, \\ g_{34} &= (\cos\vartheta_1 - 1) d_{32}d_{42} - \sin\vartheta_1 d_{31}d_{42}, \\ g_{41} &= (\cos\vartheta_1 - 1) d_{12}d_{42} + \sin\vartheta_1 d_{11}d_{42}, \\ g_{42} &= (\cos\vartheta_1 - 1) d_{22}d_{42} + \sin\vartheta_1 d_{21}d_{42}, \\ g_{43} &= (\cos\vartheta_1 - 1) d_{32}d_{42} + \sin\vartheta_1 d_{31}d_{42}, \\ g_{44} &= (\cos\vartheta_1 - 1) d_{42}^2 + 1. \end{aligned}$$

Thus, by virtue of Eqs. (15) and (17), the matrix representation of the Grover iteration G_1 defined in Eq. (18) relative to the ordered orthonormal basis $\{|\alpha_0\rangle, |\beta\rangle, |S_1\rangle, |S_1^{\perp}\rangle\}$ is computed to be

$$Qz_1 = \begin{pmatrix} Qt_{11} & Qt_{12} & Qt_{13} & Qt_{14} \\ Qt_{21} & Qt_{22} & Qt_{23} & Qt_{24} \\ Qt_{31} & Qt_{32} & Qt_{33} & Qt_{34} \\ Qt_{41} & Qt_{42} & Qt_{43} & Qt_{44} \end{pmatrix}, \quad (24)$$

with entries given by

$$\begin{aligned} Qt_{11} &= (1 - \cos\vartheta_1) d_{12}^2 + (\cos\vartheta_1 + 1) d_{11}^2 - 1 + 2\sin\vartheta_1 d_{11}d_{12}, \\ Qt_{12} &= (\cos\vartheta_1 - 1) d_{12}d_{22} - (\cos\vartheta_1 + 1) d_{11}d_{21} \\ &\quad - \sin\vartheta_1 (d_{21}d_{12} + d_{11}d_{22}), \\ Qt_{13} &= (1 - \cos\vartheta_1) d_{12}d_{32} + (\cos\vartheta_1 + 1) d_{11}d_{31} \\ &\quad + \sin\vartheta_1 (d_{31}d_{12} + d_{11}d_{32}), \\ Qt_{14} &= (1 - \cos\vartheta_1) d_{12}d_{42} + \sin\vartheta_1 d_{11}d_{42}, \\ Qt_{21} &= (1 - \cos\vartheta_1) d_{12}d_{22} + (\cos\vartheta_1 + 1) d_{11}d_{21} \\ &\quad + \sin\vartheta_1 (d_{11}d_{22} + d_{21}d_{12}), \\ Qt_{22} &= (\cos\vartheta_1 - 1) d_{22}^2 - (\cos\vartheta_1 + 1) d_{21}^2 + 1 - 2\sin\vartheta_1 d_{21}d_{22}, \\ Qt_{23} &= (1 - \cos\vartheta_1) d_{22}d_{32} + (\cos\vartheta_1 + 1) d_{21}d_{31} \\ &\quad + \sin\vartheta_1 (d_{31}d_{22} + d_{21}d_{32}), \\ Qt_{24} &= (1 - \cos\vartheta_1) d_{22}d_{42} + \sin\vartheta_1 d_{21}d_{42}, \\ Qt_{31} &= (1 - \cos\vartheta_1) d_{12}d_{32} + (\cos\vartheta_1 + 1) d_{11}d_{31} \\ &\quad + \sin\vartheta_1 (d_{11}d_{32} + d_{31}d_{12}), \\ Qt_{32} &= (\cos\vartheta_1 - 1) d_{22}d_{32} - (\cos\vartheta_1 + 1) d_{21}d_{31} \\ &\quad - \sin\vartheta_1 (d_{21}d_{32} + d_{31}d_{22}), \\ Qt_{33} &= (1 - \cos\vartheta_1) d_{32}^2 + (\cos\vartheta_1 + 1) d_{31}^2 - 1 + 2\sin\vartheta_1 d_{31}d_{32}, \\ Qt_{34} &= (1 - \cos\vartheta_1) d_{32}d_{42} + \sin\vartheta_1 d_{31}d_{42}, \\ Qt_{41} &= (1 - \cos\vartheta_1) d_{12}d_{42} + \sin\vartheta_1 d_{11}d_{42}, \\ Qt_{42} &= (\cos\vartheta_1 - 1) d_{22}d_{42} - \sin\vartheta_1 d_{21}d_{42}, \\ Qt_{43} &= (1 - \cos\vartheta_1) d_{32}d_{42} + \sin\vartheta_1 d_{31}d_{42}, \\ Qt_{44} &= (1 - \cos\vartheta_1) d_{42}^2 - 1. \end{aligned}$$

III. PERFORMANCE OF GROVER'S SEARCH ALGORITHM IN THE THREE-, FOUR-, AND ARBITRARILY HIGH-DIMENSIONAL SEARCH SPACES

In this section we shall first state and prove two theorems that are fundamental to understanding the behavior of Grover's search algorithm under the constraints (9) and (10). In the subsequent Theorem 3 we shall then answer the motivating question of how this algorithm is applicable to the cases of the search spaces of arbitrarily high dimensions.

Theorem 1 *(***Three-dimensional cases***) Let $|\mu_1\rangle$, $|\mu_2\rangle$ and $|\mu_l\rangle$ for $l = 0$ be defined as in Eqs. (15), (17) and (6), respectively, and let N be sufficiently large. Then, by repeatedly applying the Grover iteration G_1 defined in Eq. (18) to the initial superposition $|\mu_0\rangle$, the maximum success probability of Grover's search algorithm is approximately equal to $\sin^2(\omega_1/2 + \omega_2/2)$ if:*

(i) $\phi_2=\phi_1$, $\vartheta_1=|\omega_1-\omega_2|\geq 0$ *for* $\omega_1,\omega_2\neq\pi/2$, *and*

(ii) $\omega_1=\pi/2$, $\omega_2\neq\pi/2$ *or* $\omega_2=\pi/2$, $\omega_1\neq\pi/2$ *for* $\phi_1,\phi_2\in(0,\xi_0]$.

Proof: (i) It follows from Eq. (21) that if $\phi_2=\phi_1$ and

$$\vartheta_1=|\omega_1-\omega_2|\geq 0 \tag{25}$$

for $\omega_1,\omega_2\neq\pi/2$, then $\omega_2'=0$. Let us consider first the two cases of $\vartheta_1=\omega_1-\omega_2>0$, $\phi_2=\phi_1$ and $\vartheta_1=\omega_2-\omega_1>0$, $\phi_2=\phi_1$, for which the second column vector $(d_{12},d_{22},d_{32},d_{42})^T$ of the transition matrix T_1 given by Eq. (23), respectively, become

$$\left(-\cos\omega_1\cos\phi_1,-\cos\omega_1\sin\phi_1,\sin\omega_1,0\right)^T$$
$$\text{and}\quad \left(\cos\omega_1\cos\phi_1,\cos\omega_1\sin\phi_1,-\sin\omega_1,0\right)^T.$$

Both of the results above reduce Eq. (24) to

$$Qz_1'=\begin{pmatrix} Qt_{11}' & Qt_{12}' & Qt_{13}' & 0\\ Qt_{21}' & Qt_{22}' & Qt_{23}' & 0\\ Qt_{31}' & Qt_{32}' & Qt_{33}' & 0\\ 0 & 0 & 0 & -1\end{pmatrix} \equiv \begin{pmatrix} Qt_{11}' & Qt_{12}' & Qt_{13}'\\ Qt_{21}' & Qt_{22}' & Qt_{23}'\\ Qt_{31}' & Qt_{32}' & Qt_{33}'\end{pmatrix}, \tag{26}$$

where

$$\begin{aligned}
Qt_{11}' &= -\cos^2\phi_1\cos(\omega_1+\omega_2)-\sin^2\phi_1,\\
Qt_{12}' &= -\sin\phi_1\cos\phi_1\left(1-\cos(\omega_1+\omega_2)\right),\\
Qt_{13}' &= \cos\phi_1\sin(\omega_1+\omega_2),\\
Qt_{21}' &= \sin\phi_1\cos\phi_1\left(1-\cos(\omega_1+\omega_2)\right),\\
Qt_{22}' &= \sin^2\phi_1\cos(\omega_1+\omega_2)+\cos^2\phi_1,\\
Qt_{23}' &= \sin\phi_1\sin(\omega_1+\omega_2),\\
Qt_{31}' &= \cos\phi_1\sin(\omega_1+\omega_2),\\
Qt_{32}' &= -\sin\phi_1\sin(\omega_1+\omega_2),\\
Qt_{33}' &= \cos(\omega_1+\omega_2).
\end{aligned}$$

When N is chosen sufficiently large, then with the neglect of second and higher order terms of ϕ_1, the orthogonal matrix Qz_1' in Eq. (26) can be approximated as

$$Qz_1'\doteq Q_1=\begin{pmatrix} -\cos(\omega_1+\omega_2) & -\Omega_1 & \sin(\omega_1+\omega_2)\\ \Omega_1 & 1 & \Omega_1\cot\left(\frac{\omega_1+\omega_2}{2}\right)\\ \sin(\omega_1+\omega_2) & -\Omega_1\cot\left(\frac{\omega_1+\omega_2}{2}\right) & \cos(\omega_1+\omega_2)\end{pmatrix}, \tag{27}$$

where

$$\Omega_1=\phi_1\left(1-\cos(\omega_1+\omega_2)\right). \tag{28}$$

Further, the matrix Q_1 can be decomposed as

$$Q_1=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}-\Omega_1\begin{pmatrix}0&1&0\\-1&0&-\cot\left(\frac{\omega_1+\omega_2}{2}\right)\\0&\cot\left(\frac{\omega_1+\omega_2}{2}\right)&0\end{pmatrix}
+2\begin{pmatrix}-\cos^2\left(\frac{\omega_1+\omega_2}{2}\right)&0&\sin\left(\frac{\omega_1+\omega_2}{2}\right)\cos\left(\frac{\omega_1+\omega_2}{2}\right)\\0&0&0\\\sin\left(\frac{\omega_1+\omega_2}{2}\right)\cos\left(\frac{\omega_1+\omega_2}{2}\right)&0&-\sin^2\left(\frac{\omega_1+\omega_2}{2}\right)\end{pmatrix}, \tag{29}$$

which is analogous to Eq. (24) of Ref. [21].

Following the treatment in [21] and putting

$$\omega_{ave}=(\omega_1+\omega_2)/2, \tag{30}$$

we may eventually come to the result, for any positive integer j,

$$\left(Qz_1'\right)^j\doteq\begin{pmatrix}q_{11}&q_{12}&q_{13}\\q_{21}&q_{22}&q_{23}\\q_{31}&q_{32}&q_{33}\end{pmatrix}, \tag{31}$$

where

$$\begin{aligned}
q_{11}&=\cos\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\sin^2\omega_{ave}+(-1)^j\cos^2\omega_{ave},\\
q_{12}&=-\sin\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\sin\omega_{ave},\\
q_{13}&=\frac{\sin(2\omega_{ave})}{2}\left(\cos\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)+(-1)^{j+1}\right),\\
q_{21}&=\sin\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\sin\omega_{ave},\\
q_{22}&=\cos\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right),\\
q_{23}&=\sin\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\cos\omega_{ave},\\
q_{31}&=\frac{\sin(2\omega_{ave})}{2}\left(\cos\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)+(-1)^{j+1}\right),\\
q_{32}&=-\sin\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\cos\omega_{ave},\\
q_{33}&=\cos\left(\frac{j\Omega_1}{\sin\omega_{ave}}\right)\cos^2\omega_{ave}+(-1)^j\sin^2\omega_{ave}.
\end{aligned}$$

It is easily shown that after executing

$$J\left(\omega_{ave}=\omega_1/2+\omega_2/2,\Omega=\Omega_1\right)\doteq\left\lfloor\pi\sin\omega_{ave}/(2\Omega)\right\rfloor \tag{32}$$

times of Grover iteration G_1 on the initial state $|\mu_0\rangle=\cos\xi_0|\alpha_0\rangle+\sin\xi_0|\beta\rangle$, $\lfloor z\rfloor$ representing the largest integer which is smaller than z, the maximum success probability of Grover's search algorithm, defined as the square of the corresponding amplitude $\langle\beta|G_1^{J(\omega_{ave},\Omega)}|\mu_0\rangle$, is given approximately by

$$\mathbf{P}_{\max}\left(j=J\left(\omega_{ave}=\omega_1/2+\omega_2/2,\Omega=\Omega_1\right)\right)\doteq\sin^2\omega_{ave}. \tag{33}$$

So (i) is proven.

Henceforth, the maximum success probabilities of Grover's search algorithm will be denoted by $\mathbf{P}_{\max}\left(j=J\left(\omega_{ave},\Omega\right)\right)$ and the required numbers of iterations to attain them by $J\left(\omega_{ave},\Omega\right)$ for the different cases that arise in the remainder of this paper.

Turning to (ii), from Eqs. (15)-(17) we see that if $\omega_1=\pi/2$, $\omega_2\neq\pi/2$ for any $\phi_1,\phi_2\in(0,\xi_0]$, then we may substitute $|S_2\rangle$ for $|S_1\rangle$ and set $\omega_2'=0$. Consequently, the entries in the first and second columns of the transition matrix T_1 (23) now become $\tilde{d}_{11}=\cos\phi_1$, $\tilde{d}_{21}=\sin\phi_1$, $\tilde{d}_{31}=0$, $\tilde{d}_{41}=0$,

$$\begin{cases}\tilde{d}_{12}=\dfrac{\sin\omega_2\cos\phi_2-\cos\vartheta_1\cos\phi_1}{\sin\vartheta_1}\\ \tilde{d}_{22}=\dfrac{\sin\omega_2\sin\phi_2-\cos\vartheta_1\sin\phi_1}{\sin\vartheta_1},\\ \tilde{d}_{32}=\dfrac{\cos\omega_2}{\sin\vartheta_1}\end{cases}\tag{34}$$

$\tilde{d}_{42}=0$. Here $\tilde{d}_{i_1 i_2}$ $(1\leq i_1\leq 4, 1\leq i_2\leq 2)$ are used in place of $d_{i_1 i_2}$ to avoid confusion later. Hence in this case, Eq. (24) simplifies to

$$Qz_1''=\begin{pmatrix}Qt_{11}'' & Qt_{12}'' & Qt_{13}'' & 0\\ Qt_{21}'' & Qt_{22}'' & Qt_{23}'' & 0\\ Qt_{31}'' & Qt_{32}'' & Qt_{33}'' & 0\\ 0 & 0 & 0 & -1\end{pmatrix}\equiv\begin{pmatrix}Qt_{11}'' & Qt_{12}'' & Qt_{13}''\\ Qt_{21}'' & Qt_{22}'' & Qt_{23}''\\ Qt_{31}'' & Qt_{32}'' & Qt_{33}''\end{pmatrix},\tag{35}$$

where

$$\begin{aligned}Qt_{11}''&=(1-\cos\vartheta_1)\,\tilde{d}_{12}^2+(\cos\vartheta_1+1)\,\tilde{d}_{11}^2-1+2\sin\vartheta_1\tilde{d}_{11}\tilde{d}_{12},\\ Qt_{12}''&=(\cos\vartheta_1-1)\,\tilde{d}_{12}\tilde{d}_{22}-(\cos\vartheta_1+1)\,\tilde{d}_{11}\tilde{d}_{21}\\ &\quad-\sin\vartheta_1\left(\tilde{d}_{21}\tilde{d}_{12}+\tilde{d}_{11}\tilde{d}_{22}\right),\\ Qt_{13}''&=(1-\cos\vartheta_1)\,\tilde{d}_{12}\tilde{d}_{32}+\tilde{d}_{11}\tilde{d}_{32}\sin\vartheta_1,\\ Qt_{21}''&=(1-\cos\vartheta_1)\,\tilde{d}_{12}\tilde{d}_{22}+(\cos\vartheta_1+1)\,\tilde{d}_{11}\tilde{d}_{21}\\ &\quad+\sin\vartheta_1\left(\tilde{d}_{11}\tilde{d}_{22}+\tilde{d}_{21}\tilde{d}_{12}\right),\\ Qt_{22}''&=(\cos\vartheta_1-1)\,\tilde{d}_{22}^2-(\cos\vartheta_1+1)\,\tilde{d}_{21}^2+1-2\sin\vartheta_1\tilde{d}_{21}\tilde{d}_{22},\\ Qt_{23}''&=(1-\cos\vartheta_1)\,\tilde{d}_{22}\tilde{d}_{32}+\tilde{d}_{21}\tilde{d}_{32}\sin\vartheta_1,\\ Qt_{31}''&=(1-\cos\vartheta_1)\,\tilde{d}_{12}\tilde{d}_{32}+\tilde{d}_{11}\tilde{d}_{32}\sin\vartheta_1,\\ Qt_{32}''&=(\cos\vartheta_1-1)\,\tilde{d}_{22}\tilde{d}_{32}-\tilde{d}_{21}\tilde{d}_{32}\sin\vartheta_1,\\ Qt_{33}''&=(1-\cos\vartheta_1)\,\tilde{d}_{32}^2-1.\end{aligned}$$

For clarity, we consider first the case $\phi_2\neq\phi_1$, $\omega_2\in(0,\omega')$ with $\omega'\ll\pi/2$. The normalization $\sum_{i_1=1}^{3}\tilde{d}_{i_1 2}^2=1$ with $\tilde{d}_{i_1 2}$ given by Eqs. (34) yields

$$\cos\vartheta_1=\sin\omega_2\cos(\phi_2-\phi_1)\tag{36}$$

that holds for all $\omega_2\in(0,\pi/2]$ and all $\phi_1,\phi_2\in(0,\xi_0]$, whence $\cos\vartheta_1\doteq\sin\omega_2$, that is, $\vartheta_1\doteq\pi/2-\omega_2\gg 0$, in the case when N is sufficiently large. It follows from this that $\tilde{d}_{12}\doteq 0$, $\tilde{d}_{22}\doteq(\phi_2-\phi_1)\cot\vartheta_1$ ($\tilde{d}_{22}^2\doteq 0$ for $\vartheta_1\gg 0$), $\tilde{d}_{32}\doteq 1$. With use of these and recognizing $\tilde{d}_{11}\doteq 1$, $\tilde{d}_{21}\doteq\phi_1$ ($\tilde{d}_{21}^2\doteq 0$), we can approximately write the orthogonal matrix Qz_1'' in Eq. (35) as

$$\begin{aligned}Qz_1''\doteq Q_2&=\begin{pmatrix}\cos\vartheta_1 & -\Omega_2 & \sin\vartheta_1\\ \Omega_2 & 1 & \Omega_2\tan(\vartheta_1/2)\\ \sin\vartheta_1 & -\Omega_2\tan(\vartheta_1/2) & -\cos\vartheta_1\end{pmatrix}\\ &=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}-\Omega_2\begin{pmatrix}0&1&0\\-1&0&-\tan(\vartheta_1/2)\\0&\tan(\vartheta_1/2)&0\end{pmatrix}\\ &\quad+2\begin{pmatrix}-\sin^2(\vartheta_1/2)&0&\sin(\vartheta_1/2)\cos(\vartheta_1/2)\\0&0&0\\ \sin(\vartheta_1/2)\cos(\vartheta_1/2)&0&-\cos^2(\vartheta_1/2)\end{pmatrix},\end{aligned}\tag{37}$$

where

$$\Omega_2=\phi_1+\phi_2\cos\vartheta_1.\tag{38}$$

This also applies to $\phi_2\neq\phi_1$, $\omega_2\in[\omega',\pi/2)$ and to $\phi_2=\phi_1$, $\omega_2\in(0,\pi/2)$ corresponding, respectively, to $\vartheta_1\doteq\pi/2-\omega_2$ and $\vartheta_1=\pi/2-\omega_2$ in accordance with Eq. (36). For $\omega_2\in(0,\pi/2)$ we let

$$\omega_{ave}=\omega_{ave}'=\pi/2-\vartheta_1/2$$
$$\Rightarrow\omega_{ave}=\omega_{ave}'\begin{cases}=\pi/4+\omega_2/2 & \text{for }\phi_2=\phi_1\\ \doteq\pi/4+\omega_2/2 & \text{otherwise.}\end{cases}$$

Then Q_2 in Eq. (37) has the form of Q_1 in Eq. (29), and therefore properties (32) and (33) hold for the case discussed above as well, namely

$$J\left(\omega_{ave}=\omega_{ave}',\Omega=\Omega_2\right)\doteq\left\lfloor\pi\sin\omega_{ave}/(2\Omega)\right\rfloor,\tag{39}$$

$$\mathbf{P}_{\max}\left(j=J\left(\omega_{ave}=\omega_{ave}',\Omega=\Omega_2\right)\right)\doteq\sin^2\omega_{ave}.\tag{40}$$

The same argument allows the proof of the cases $\omega_1=\pi/2$, $\omega_2\in(\pi/2,\pi)$ and $\omega_1\neq\pi/2$, $\omega_2=\pi/2$ to be adapted to give the analogue formulations. So (ii) is proven. □

Theorem 2 (**Four-dimensional case**) *Let $|\mu_0\rangle$, $|\mu_1\rangle$, $|\mu_2\rangle$, and N be such as in Theorem 1, and let $\phi_2\neq\phi_1$ in $(0,\xi_0]$. Then the property stated in Theorem 1 also holds under the restrictive condition*

$$\left(\frac{\omega_2'\cos\omega_2}{\cos(\omega_2/2-\omega_1/2)}\right)^2\to 0$$

for $\omega_2'>0$, as defined in Eq. (14), and $\omega_1,\omega_2\in(0,\pi/2)\cup(\pi/2,\pi)$.

Proof: As we have seen in case (i) of Theorem 1, $\omega_2'=0$ for $\omega_1,\omega_2\neq\pi/2$ when $\phi_2=\phi_1$, since in this case condition (25) holds automatically. This implies that if we fix ϕ_1 and ϕ_2 with $\phi_1\neq\phi_2$, then $|S_1\rangle$ and $|S_2\rangle$ in Eqs. (11), originating from the deviations of $|\mu_1\rangle$ and $|\mu_2\rangle$ from the two-dimensional subspace L_0, are invariant with respect to any change of ω_1 and ω_2 , which leaves the angle $\omega_2'\geq 0$ between $|S_1\rangle$ and

$|S_2\rangle$ unaltered. Let us mention parenthetically here that for $\omega_1,\omega_2 \neq \pi/2$, the equality

$$\cos\vartheta_1 = \sin\omega_1 \sin\omega_2 \cos(\phi_2-\phi_1) + \cos\omega_1\cos\omega_2$$

with $\phi_1 \neq \phi_2$, from Eq. (21), is also responsible for producing a vanishing angle ω_2'.

To estimate ω_2' for $\omega_1,\omega_2 \neq \pi/2$ in the case of $\phi_1 \neq \phi_2$, we first put $\omega_2 = \omega_1 \in (0,\pi/2)\cup(\pi/2,\pi)$ and we then subtract $\cos\omega_2'$ from both sides of Eq. (21). This gives

$$\cos\vartheta - \cos\omega_2' = \sin^2\omega_1\left(\cos(\phi_2-\phi_1) - \cos\omega_2'\right), \qquad (41)$$

where we identify ϑ with $\vartheta_{1(\omega_2=\omega_1\neq\pi/2,\phi_1\neq\phi_2)}$ for notational convenience. Since $0<\sin^2\omega_1<1$, it follows that

(*a*) if $\vartheta = \omega_2'$, $|\phi_2-\phi_1| = \omega_2'$,

(*b*) if $\vartheta < \omega_2'$, then $|\phi_2-\phi_1| < \omega_2'$ and $|\phi_2-\phi_1| < \vartheta$, i.e. $|\phi_2-\phi_1| < \vartheta < \omega_2'$, and

(*c*) if $\vartheta > \omega_2' \geq 0$, then $|\phi_2-\phi_1| > \omega_2'$ and $|\phi_2-\phi_1| > \vartheta$, i.e. $|\phi_2-\phi_1| > \vartheta > \omega_2' \geq 0$.

If case (*b*) occurs, we recast Eq. (41) in the form

$$\frac{\cos\vartheta}{\cos(\phi_2-\phi_1)} = \sin^2\omega_1 + \cos^2\omega_1\frac{\cos\omega_2'}{\cos(\phi_2-\phi_1)}. \qquad (42)$$

In this situation it is easily seen that both ϑ and ω_2' tend to $|\phi_2-\phi_1| \neq 0$ as $\omega_2=\omega_1 \to \pi/2$, while ω_2' does not depend on ω_1 and ω_2 with the given ϕ_1 and ϕ_2, as explained above. We thus conclude that the maximum possible value of the angle ω_2' in question is in the close vicinity of $|\phi_2-\phi_1|$. Note that this fact is not limited to cases where N is large, but rather holds for general N. Hence, combining this result with those of (*a*) and (*c*), under the conditions stated in Theorem 2 we have that (*1*) $\vartheta_1 \doteq \omega_2-\omega_1$, $\pi > \omega_2 \geq \omega_1 > 0$ and (*2*) $\vartheta_1 \doteq \omega_1-\omega_2$, $0<\omega_2<\omega_1<\pi$ with $\omega_1,\omega_2\neq\pi/2$ in both cases according to Eq. (21).

First for (*1*), using the definitions of $d_{i_1 i_2}$ $(1\leq i_1\leq 4, 1\leq i_2\leq 2)$ given in Eq. (23), Eq. (24) can be approximately reduced to

$$Qz_1 \doteq Qs = \begin{pmatrix} Qs_{11} & Qs_{12} & Qs_{13} & Qs_{14} \\ Qs_{21} & Qs_{22} & Qs_{23} & Qs_{24} \\ Qs_{31} & Qs_{32} & Qs_{33} & Qs_{34} \\ Qs_{41} & Qs_{42} & Qs_{43} & Qs_{44} \end{pmatrix}, \qquad (43)$$

where

$$Qs_{11} = -\cos(\omega_1+\omega_2),$$
$$Qs_{12} = -\kappa_1(\phi_1\sin\omega_1 + \phi_2\sin\omega_2),$$
$$Qs_{13} = \sin(\omega_1+\omega_2), \qquad Qs_{14} = \kappa_1\omega_2'\cos\omega_2,$$
$$Qs_{21} = \kappa_1(\phi_1\sin\omega_1+\phi_2\sin\omega_2), \qquad Qs_{22} = 1,$$
$$Qs_{23} = \kappa_2(\phi_1\sin\omega_1+\phi_2\sin\omega_2), \qquad Qs_{24} = 0,$$
$$Qs_{31} = \sin(\omega_1+\omega_2),$$
$$Qs_{32} = -\kappa_2(\phi_1\sin\omega_1+\phi_2\sin\omega_2),$$
$$Qs_{33} = \cos(\omega_1+\omega_2), \qquad Qs_{34} = \kappa_2\omega_2'\cos\omega_2,$$
$$Qs_{41} = \kappa_1\omega_2'\cos\omega_2, \qquad Qs_{42} = 0,$$
$$Qs_{43} = \kappa_2\omega_2'\cos\omega_2, \qquad Qs_{44} = -1,$$

where $\kappa_1 = \sin\omega_1 + \tan(\vartheta_1/2)\cos\omega_1$ and $\kappa_2 = \cos\omega_1 - \tan(\vartheta_1/2)\sin\omega_1$. Similarly, for (*2*), we get

$$Qz_1 \doteq Qs' = \begin{pmatrix} Qs'_{11} & Qs'_{12} & Qs'_{13} & Qs'_{14} \\ Qs'_{21} & Qs'_{22} & Qs'_{23} & Qs'_{24} \\ Qs'_{31} & Qs'_{32} & Qs'_{33} & Qs'_{34} \\ Qs'_{41} & Qs'_{42} & Qs'_{43} & Qs'_{44} \end{pmatrix}, \qquad (44)$$

where

$$Qs'_{11} = -\cos(\omega_1+\omega_2),$$
$$Qs'_{12} = -\kappa_1'(\phi_1\sin\omega_1+\phi_2\sin\omega_2),$$
$$Qs'_{13} = \sin(\omega_1+\omega_2), \qquad Qs'_{14} = \kappa_1'\omega_2'\cos\omega_2,$$
$$Qs'_{21} = \kappa_1'(\phi_1\sin\omega_1+\phi_2\sin\omega_2), \qquad Qs'_{22} = 1,$$
$$Qs'_{23} = \kappa_2'(\phi_1\sin\omega_1+\phi_2\sin\omega_2), \qquad Qs'_{24} = 0,$$
$$Qs'_{31} = \sin(\omega_1+\omega_2),$$
$$Qs'_{32} = -\kappa_2'(\phi_1\sin\omega_1+\phi_2\sin\omega_2),$$
$$Qs'_{33} = \cos(\omega_1+\omega_2), \qquad Qs'_{34} = \kappa_2'\omega_2'\cos\omega_2,$$
$$Qs'_{41} = \kappa_1'\omega_2'\cos\omega_2, \qquad Qs'_{42} = 0,$$
$$Qs'_{43} = \kappa_2'\omega_2'\cos\omega_2, \qquad Qs'_{44} = -1,$$

where $\kappa_1' = \sin\omega_1 - \tan(\vartheta_1/2)\cos\omega_1$ and $\kappa_2' = \cos\omega_1 + \tan(\vartheta_1/2)\sin\omega_1$.

Note that

$$\chi^2 = \left(\frac{\omega_2'\cos\omega_2}{\cos(\omega_2/2-\omega_1/2)}\right)^2 \to 0 \qquad (45)$$

for both cases (*1*) and (*2*), owing to the relations $(Qs_{41})^2 + (Qs_{42})^2 + (Qs_{43})^2 + (Qs_{44})^2 \to 1$ and $(Qs'_{41})^2 + (Qs'_{42})^2 + (Qs'_{43})^2 + (Qs'_{44})^2 \to 1$. Whether we choose to work with Qs or Qs', Qz_1 can be approximately written in terms of the following decomposition:

$$Qz_1 \doteq \begin{pmatrix} B & O_1 \\ O_2 & -1 \end{pmatrix} + \chi\begin{pmatrix} O & A_1 \\ A_2 & 0 \end{pmatrix}, \qquad (46)$$

where O denotes a 3 by 3 zero matrix, $A_2 = (\sin(\omega_1/2+\omega_2/2), 0, \cos(\omega_1/2+\omega_2/2))$, $A_1 = (A_2)^T$, $O_2 = (0,0,0)$, $O_1 = (O_2)^T$, and

$$B = I_{3\times3} - \Omega_3 B_1 + 2B_2 \qquad (47)$$

where $I_{3\times3}$ is a 3 by 3 identity matrix,

$$B_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & -\cot\left(\frac{\omega_1+\omega_2}{2}\right) \\ 0 & \cot\left(\frac{\omega_1+\omega_2}{2}\right) & 0 \end{pmatrix},$$

$$B_2 = \begin{pmatrix} -\cos^2\left(\frac{\omega_1+\omega_2}{2}\right) & 0 & \sin\left(\frac{\omega_1+\omega_2}{2}\right)\cos\left(\frac{\omega_1+\omega_2}{2}\right) \\ 0 & 0 & 0 \\ \sin\left(\frac{\omega_1+\omega_2}{2}\right)\cos\left(\frac{\omega_1+\omega_2}{2}\right) & 0 & -\sin^2\left(\frac{\omega_1+\omega_2}{2}\right) \end{pmatrix},$$

$$\Omega_3 = \frac{\sin(\omega_1/2+\omega_2/2)}{\cos(\omega_2/2-\omega_1/2)}(\phi_1\sin\omega_1+\phi_2\sin\omega_2). \qquad (48)$$

For all integers $j > 1$, we can evaluate the matrix Qz_1^j as

$$Qz_1^j \doteq \begin{pmatrix} B^j & O_1 \\ O_2 & (-1)^j \end{pmatrix} + \chi \begin{pmatrix} O & (B - I_{3\times3})^{j-1} A_1 \\ A_2 (B - I_{3\times3})^{j-1} & 0 \end{pmatrix} = \begin{pmatrix} B^j & O_1 \\ O_2 & (-1)^j \end{pmatrix} + \begin{pmatrix} O & \left(\chi(-\Omega_3 B_1 + 2B_2)^{j-1}\right) A_1 \\ A_2 \left(\chi(-\Omega_3 B_1 + 2B_2)^{j-1}\right) & 0 \end{pmatrix} \doteq \begin{pmatrix} B^j & O_1 \\ O_2 & (-1)^j \end{pmatrix} + \begin{pmatrix} O & O_1 \\ O_2 & 0 \end{pmatrix} \equiv B^j, \quad (49)$$

where, in the first step, we have used successively the restriction (45), then Eq. (47) and the properties $B_1 B_2 = B_2 B_1 = O$, $(B_2)^2 = -B_2$, and finally the relation $(A_2 B_2)^T = B_2 A_1 = O_1$. By comparing the decomposition (47) to (29), it follows, on account of Eq. (49), that

$$J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_3) \doteq \left\lfloor \pi \sin\omega_{ave}/(2\Omega) \right\rfloor, \quad (50)$$

$$\mathbf{P}_{\max}(j = J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_3)) \doteq \sin^2 \omega_{ave}. \quad (51)$$

Theorem 2 follows. □

We now consider the removal of the restrictions (9)-(10), and without loss of generality allow the perturbations $\Delta W_0, \Delta W_1, \Delta W_2, \cdots, \Delta W_{2j-1}, \Delta W_{2j}$ in Eq. (3) to be stochastic as long as the assumption (8) holds. Then, the dimension n_j of the search space to which $|\alpha_0\rangle, |\beta\rangle, |\mu_1\rangle, |\mu_2\rangle, \cdots, |\mu_{2j-1}\rangle, |\mu_{2j}\rangle$ belong progressively goes up as j increases in general (but is ultimately less than or equal to N), whereas for each $j > 1$, with respect to the ordered orthonormal basis $\{|\alpha_0\rangle, |\beta\rangle, |S_{2j-1}\rangle, |S_{2j-1}^{\perp}\rangle\}$, we can individually compute the matrix representation Qz_j of G_j that is defined in Eq. (4), with parameters $\phi_{2j-1}, \phi_{2j}, \omega_{2j-1}, \omega_{2j}, \omega'_{2j}, \vartheta_j$ defined as in the case of $j = 1$. Obviously, every $Qz_{j>1}$ has the same form as Qz_1. We shall show the following:

Theorem 3 *(***Arbitrarily high-dimensional cases***)* *Let the initial state $|\mu_0\rangle$ of the quantum system evolve according to unitary dynamics $F_j = \prod_{k=1}^{j} Qz_k(\phi_{2k-1}, \phi_{2k}, \omega_{2k-1}, \omega_{2k}, \omega'_{2k}, \vartheta_k)$ under consideration above, and let $|\mu_1\rangle, |\mu_2\rangle \notin L_0$ and $\omega'_2 \neq 0$ be as in definition (14). If N is sufficiently large and the condition*

$$\omega_{ave} = \omega_1/2 + \omega_2/2 \approx \omega_3/2 + \omega_4/2 \approx \cdots \approx \omega_{2j-1}/2 + \omega_{2j}/2 \quad (52)$$

imposes the following constraint on F_j:

$$\left(\frac{\omega'_{2k}\cos\omega_{2k}}{\cos(\omega_{2k}/2 - \omega_{2k-1}/2)}\right)^2 \to 0 \quad \textit{when } \omega'_{2\le 2k\le 2j} \neq 0, \quad (53)$$

then the desired state $|\beta\rangle$ can be found with maximum success probability approximately equal to $\sin^2\omega_{ave}$ for search spaces of any finite dimension.

Proof: Letting N be sufficiently large and letting $j > 1$ be given, it follows as in the proof of Theorem 2 that when $|S_{2j'-1}\rangle \neq |S_1\rangle$, $j' = 2, \cdots, j$, $\langle S_{2j'-1} \mid S_1\rangle \doteq 1$, and hence that $|S_{2j'-1}\rangle \doteq |S_1\rangle$. Similarly, if $|S_{2j'}\rangle \neq |S_2\rangle$ then $|S_{2j'}\rangle \doteq |S_2\rangle$ for all $j' = 2, \cdots, j$. Therefore, for an arbitrary $4 < n_j \le N$, the resulting state $|\psi'_j\rangle$ (3) of the quantum system can be approximately described as

$$|\psi'_j\rangle \doteq \left(\prod_{k=1}^{j} Qz_1(\phi_{2k-1}, \phi_{2k}, \omega_{2k-1}, \omega_{2k}, \omega'_{2k}, \vartheta_k)\right) |\mu_0\rangle. \quad (54)$$

For typographical convenience we shall abbreviate $Qz_1(\phi_{2k-1}, \phi_{2k}, \omega_{2k-1}, \omega_{2k}, \omega'_{2k}, \vartheta_k)$ to $Qz_1|A_k$ with label $A_k = \{\phi_{2k-1}, \phi_{2k}, \omega_{2k-1}, \omega_{2k}, \omega'_{2k}, \vartheta_k\}$ in what follows. Under the conditions (52) and (53), repeating the analogous steps to Eq. (49) yields

$$\prod_{k=1}^{j} Qz_1|A_k \approx \begin{pmatrix} \prod_{k=1}^{j} B|A_k & O_1 \\ O_2 & (-1)^j \end{pmatrix} \equiv \prod_{k=1}^{j} B|A_k, \quad (55)$$

where the matrices $B|A_{k\neq1}$ are defined exactly as the matrix $B = B|A_{k=1}$ given in Eq. (47). Then by closely mimicking the derivation in Ref. [21] again, ultimately we can conveniently substitute

$$\Omega_4 = \frac{1}{j}\sum_{k=1}^{j} \Omega_3|A_k \quad (56)$$

for Ω_1 in the elements of the matrix $(Qz'_1)^j$ given in Eq. (31) to obtain

$$\prod_{k=1}^{j} B|A_k \doteq \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix}, \quad (57)$$

where

$$t_{11} = \cos\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\sin^2\omega_{ave} + (-1)^j\cos^2\omega_{ave},$$

$$t_{12} = -\sin\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\sin\omega_{ave},$$

$$t_{13} = \frac{\sin(2\omega_{ave})}{2}\left(\cos\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right) + (-1)^{j+1}\right),$$

$$t_{21} = \sin\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\sin\omega_{ave},$$

$$t_{22} = \cos\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right),$$
$$t_{23} = \sin\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\cos\omega_{ave},$$
$$t_{31} = \frac{\sin(2\omega_{ave})}{2}\left(\cos\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right) + (-1)^{j+1}\right),$$
$$t_{32} = -\sin\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\cos\omega_{ave},$$
$$t_{33} = \cos\left(\frac{j\Omega_4}{\sin\omega_{ave}}\right)\cos^2\omega_{ave} + (-1)^j\sin^2\omega_{ave}.$$

Evidently, for the case we are considering, it can be still manipulated in exactly the same way as done below Eq. (31) as to lead to

$$J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_4) \doteq \left\lfloor \pi\sin\omega_{ave}/(2\Omega) \right\rfloor, \tag{58}$$

$$\mathbf{P}_{\max}(j = J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_4)) \doteq \sin^2\omega_{ave}, \tag{59}$$

thereby completing the proof of Theorem 3. □

IV. CONCLUSIONS

We have studied the dynamical behavior of Grover's search algorithm by imposing the random perturbations $\Delta W_0, \Delta W_1, \Delta W_2, \cdots, \Delta W_{2j-1}, \Delta W_{2j}$ on the respective Walsh-Hadamard transformations W appearing in Eq. (2). One of the main consequences of this paper is that it reveals the basic property: for all sufficiently large N, if $|S_{l_1}\rangle \neq |S_{l_2}\rangle$, $l_1, l_2 \in \{1, \cdots, 2j\}$, then $|S_{l_1}\rangle \doteq |S_{l_2}\rangle$. This property will become more transparent to intuition if we understand it from the point of view of geometric interpretation. Whence, under the conditions (52) and (53), we have derived both the maximum success probabilities of Grover's search algorithm $\mathbf{P}_{\max}(j = J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_4)) \doteq \sin^2\omega_{ave}$ and the corresponding numbers of iterations $J(\omega_{ave} = \omega_1/2 + \omega_2/2, \Omega = \Omega_4) \doteq \left\lfloor \pi\sin\omega_{ave}/(2\Omega) \right\rfloor$, applicable to search spaces of arbitrary dimension. As is easily seen from the general formula of $\mathbf{P}_{\max}$ given above, setting $\Delta W_0 = 0$ and $\sum_{l_1=1}^{2j}\Delta W_{l_1} = 0$ for small perturbations ΔW_{l_1} that just engender either $\omega_{l_1} = \pi/2 - \varepsilon_{l_1}$ ($\Delta W_{l_1} > 0$) or $\omega_{l_1} = \pi/2 + \varepsilon_{l_1}$ ($\Delta W_{l_1} < 0$) with small angles $\varepsilon_{l_1} > 0$ is equivalent to completing the substantiation of Grover's verdict in Ref. [15].

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