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Phase matching condition for quantum search with a generalized initial state

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Abstract

We present a general phase matching condition for the quantum search algorithm with arbitrary unitary transformation and arbitrary phase rotations in the case of a general initial state. We show by an explicit expression that the phase matching condition depends both on the unitary transformation U and the initial state. We show that several phase conditions previously discussed in the literature are special cases of this general one, which clarifies the question of which condition should be regarded as exact. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Grover's quantum search algorithm [1] is one of the most important developments in quantum computation. For searching a marked state in an unordered list, it achieves quadratic speedup over classical search algorithms. In Grover's original paper [1], each search step consists of two phase inversions and two Hadmard–Walsh transformations, and the initial state is an even distribution of the basis states. There have been several generalizations of the Grover algorithm. For instance, people have studied the cases with (1) more than one marked item [2]; (2) an arbitrary unitary transformation instead of the Hadmard–Walsh transformation [2]; (3) arbitrary initial distributions [3,4]; (4) arbitrary phase rotations [6,7]; and (5) arbitrarily entangled initial distribution [8].

Arbitrary phase quantum searching has been extensively studied by our group. It was found that arbitrary phase rotation of the marked state alone cannot be used for a quantum search [6]. It was later demonstrated [7] by an approximate treatment that a useful quantum search algorithm can be constructed if and only if the two phase rotations

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are equal, i.e., $\theta = \phi$ (θ and ϕ are the phase rotation angles for the $|0\rangle$ state and the marked state, respectively). It is important that this phase matching condition should be satisfied during a searching process, because the systematic error induced by phase mismatching is the dominant gate imperfection in the Grover algorithm [9], and the error tolerance in phase mismatching is of the order $O(1/\sqrt{N})$. By the isomorphism between $SU(2)$ and $SO(3)$ group, an $SO(3)$ picture for the quantum search algorithm has been established [10]. The advantage of this picture is that one can use simple geometrical method to treat quantum searching problems, even for cases where application of an analytical method is difficult. In this picture, a quantum search is described as a series of rotations in a 3-dimensional space. State vector is represented by a polarization vector. The marked item corresponds to a point in the z-axis $(x, y, z) = (0, 0, 1)$ in space. The task of a quantum search is to rotate the polarization vector, initially lying near $(0, 0, -1)$, to the target point $(0, 0, 1)$. During the searching process, the 3-dimensional state vector (polarization vector) spans a cone in space, and the tip of the polarization vector draws a circle in this cone. If the target point lies on this circle, the searching process can find the marked state. Using this $SO(3)$ picture, it was proven that the phase matching requirement $\theta = \phi$, which was obtained earlier through an approximation [7], is an exact condition. Recently, this phase matching condition has been demonstrated in a 2-qubit system by the liquid NMR technique [11].

Arbitrary phases have recently received much attention. Two papers have been published in Physical Review A, addressing particularly this issue [4,12]. In Ref. [12], Høyer discussed arbitrary phase rotations in quantum amplitude amplification, a generalization of Grover's quantum search algorithm. He obtained a phase condition $\tan(\phi/2) = \tan(\theta/2)(1 - 2a)$, where a is the success probability of the search algorithm. Using this phase condition, Høyer constructed a quantum algorithm that searches a marked state with certainty. He also confirmed that the phase error tolerance is the order $O(1/\sqrt{N})$. By considering $\theta = \phi$ as an approximation to his phase condition, he can obtain our main results in Refs. [6,7,9,10]. Since a is of the order of $1/N$, the difference between Høyer condition and our condition $\theta = \phi$ is very small. However, Høyer claimed [12] that $\tan(\phi/2) = \tan(\theta/2)(1 - 2a)$ is an exact phase condition and $\theta = \phi$ is only an approximate one. In another development, Biham et al. [4] studied the arbitrary phase rotations in a quantum search algorithm that allows arbitrary phase rotations and arbitrary initial distribution using recursion relations. In their study, they found that in order for the algorithm to apply, the two rotation angles must be equal. The phase error tolerance in Ref. [4] is found also to be the order $O(1/\sqrt{N})$. In a recent paper [5], Li et al. studied the mathematical aspects of quantum searching with arbitrary phase rotations and discussed the different effects of the rotation angles on the amplitude of the marked state. It also showed that the phase matching condition $\theta = \phi$ gives the maximal success probability.

Although the main conclusions of these papers are similar, there is an apparent contradiction in the exact phase matching condition with arbitrary phases in a quantum search algorithm. In this Letter, we will solve this paradox. This apparent paradox arises from the fact that the dependence of the phase matching condition on the initial state (or quantum database) has thus far ignored in most literature. Usually the initial state is taken as $U|0\rangle$, where U is the unitary transformation in the quantum search algorithm (see Section 2 for more details). The phase matching condition $\theta = \phi$ is derived by using this quantum database. In Høyer's paper, though he started from such an initial state, he has also made certain processing to the initial state and thus his true quantum database is different from $U|0\rangle$. This solves the paradox that both our phase matching condition and Høyer's matching condition are exact. More importantly, we have found a phase matching condition for for a generalized initial state (quantum database). Instead of $U|0\rangle$, the generalized initial state is an arbitrary superposition of $|1\rangle$ and $|2\rangle$, where

$$|1\rangle = \frac{1}{\sin\beta}\left(\sum_k |\tau_k\rangle\langle\tau_k|\right)U|0\rangle, \qquad |2\rangle = \frac{1}{\cos\beta}\left(\sum_{i\neq\tau} |i\rangle\langle i|\right)U|0\rangle, \qquad \sin\beta = \sqrt{\sum_k |U_{\tau_k 0}|^2}.$$

We shall also point out that other phase conditions are special cases of the general phase matching condition derived in this Letter.

The Letter is organized as follows. After this introduction, we briefly review the structure of a quantum search problem in Section 2. Here we particularly divide a quantum search algorithm into two parts: the quantum searching engine and the quantum database (the initial state). In this way, one can see clearly the dependence of the phase

matching condition on the unitary transformation U and the initial distribution. This detailed dependence was ignored in previous discussions because the initial state has been taken as $U|0\rangle$. In Section 3, we give the general phase matching condition using the $SO(3)$ quantum searching picture. The advantage of this $SO(3)$ picture is the ease to treat quantum search problems in a simple geometrical picture. It is particularly useful in solving this problem. In Section 4, we demonstrate our general phase matching condition by several known examples. In Section 5, we discuss the influence of the phases on the computational complexity of the searching problem. Finally, a summary is given in Section 6.

2. Structure of a quantum search algorithm

Let us review two basic aspects in a quantum search problem. First, one must have a searching operation (we call it a search engine hereafter). Combining various generalizations, we can write a general quantum searching engine as the following operator:

$$Q = -U I_\gamma U^{-1} I_\tau, \tag{1}$$

where

$$I_\tau = I + \left(e^{i\phi} - 1\right) \sum_k |\tau_k\rangle\langle\tau_k|, \qquad I_\gamma = I + \left(e^{i\theta} - 1\right)|\gamma\rangle\langle\gamma|.$$

Usually $|\gamma\rangle$ is chosen as $|0\rangle \equiv |0\ldots0\rangle$. Here $|\tau_k\rangle$ is a marked state, and the summation runs over all the marked states. Thus, this quantum search engine can deal with cases with more than one marked state. We see that a quantum search engine is determined by the following factors: a unitary transformation U, two phase rotations and the marked states.

Secondly, there must be a quantum database: the initial distribution $|\psi_0\rangle$. This part is independent of the searching engine: for a given searching engine, the initial state may be prepared in various ways. However, a special form of the initial state makes the search problem simple. It was found in Refs. [2,13] that the space span by $|1\rangle$ and $|2\rangle$ is invariant under the action of the quantum searching operator Q. If the initial state is a superposition of these two state vectors, then the quantum search problem can be dealt with in a 2-dimensional space [2,14].

In the literature, nearly all the initial distribution is chosen as

$$U|0\rangle = \sum_i |i\rangle\langle i|U|0\rangle = \sum_k |\tau_k\rangle\langle\tau_k|U|0\rangle + \sum_{i\neq\tau} |i\rangle\langle i|U|0\rangle = \sin\beta|1\rangle + \cos\beta|2\rangle, \tag{2}$$

where

$$|1\rangle = \frac{1}{\sin\beta}\left(\sum_k |\tau_k\rangle\langle\tau_k|\right)U|0\rangle = \frac{1}{\sin\beta}\sum_k |\tau_k\rangle U_{\tau_k 0}, \qquad |2\rangle = \frac{1}{\cos\beta}\left(\sum_{i\neq\tau} |i\rangle\langle i|\right)U|0\rangle = \frac{1}{\cos\beta}\sum_{i\neq\tau} |i\rangle U_{i0},$$

$$\sin\beta = \sqrt{\sum_k |U_{\tau_k 0}|^2}.$$

For instance, in the Grover algorithm, the evenly distributed initial state takes the form

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle = \frac{1}{\sqrt{N}}|1\rangle + \sqrt{\frac{N-1}{N}}|2\rangle.$$

Of course, the form of the initial state may take a more general form. For instance, using the standard Grover searching engine where the unitary transformation is chosen as the Hadmard–Walsh transformation, the quantum search problem with arbitrary initial state was studied in Ref. [3]. This was generalized to a quantum search engine

with arbitrary phases and arbitrary unitary transformation in Ref. [4]. In that case, the amplitudes of the marked states and unmarked states are not tied together during a searching process, and one no longer has a 2-dimensional rotation structure.

In this Letter, we restrict ourselves to the case where the initial state is an arbitrary superposition of $|1\rangle$ and $|2\rangle$ (we refer this case as quasi-arbitrary initial distribution, to distinguish this from that in Refs. [3,4]). The action of operator Q on the two basis states are [7,12,15]

$$Q \begin{bmatrix} |1\rangle \\ |2\rangle \end{bmatrix} = \begin{bmatrix} -e^{i\phi}(1 + (e^{i\theta} - 1)\sin^2 \beta) & -(e^{i\theta} - 1)\sqrt{\sin^2 \beta(1 - \sin^2 \beta)} \\ -e^{i\phi}(e^{i\theta} - 1)\sin \beta \cos \beta & -e^{i\theta} + (e^{i\theta} - 1)\sin^2 \beta \end{bmatrix} \begin{bmatrix} |1\rangle \\ |2\rangle \end{bmatrix}.$$

Within this $U(2)$-formalism, after dropping a global phase factor, the initial state can be written most generally as

$$|\psi_0\rangle = \sin\theta_0 |1\rangle + \cos\theta_0 e^{i\delta} |2\rangle. \tag{3}$$

3. General phase matching condition

We now derive, in the $SO(3)$ picture, the phase matching requirement of the quantum searching engine (1) with the initial state (3). The essence of the $SO(3)$ picture is that the quantum search operator in (1) is thought as a rotation operation in a 3-dimensional space. Explicitly, the matrix representing operator Q in the basis span by $|1\rangle$ and $|2\rangle$ can be represented by a rotation in 3 dimensions,

$$R_Q = \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{bmatrix}, \tag{4}$$

where

$$R_{11} = \cos\phi\left(\cos^2 2\beta \cos\theta + \sin^2 2\beta\right) + \cos 2\beta \sin\theta \sin\phi, \qquad R_{12} = \cos\phi \sin\theta \cos 2\beta - \cos\theta \sin\phi,$$

$$R_{13} = -\cos\phi \sin 4\beta \sin^2 \frac{\theta}{2} + \sin 2\beta \sin\theta \sin\phi,$$

$$R_{21} = -\cos 2\beta \cos\phi \sin\theta + \left(\cos^2 \frac{\theta}{2} - \cos 4\beta \sin^2 \frac{\theta}{2}\right)\sin\phi, \qquad R_{22} = \cos\theta \cos\phi + \cos 2\beta \sin\theta \sin\phi,$$

$$R_{23} = -\cos\phi \sin 2\beta \sin\theta - \sin 4\beta \sin^2 \frac{\theta}{2} \sin\phi,$$

$$R_{31} = -\sin 4\beta \sin^2 \frac{\theta}{2}, \qquad R_{32} = \sin 2\beta \sin\theta, \qquad R_{33} = \cos^2 2\beta + \cos\theta \sin^2 2\beta.$$

This $SO(3)$ transformation corresponds to a rotation about an axis $\vec{l}$ through a rotation angle α, which can be expressed as

$$\vec{l} = \begin{bmatrix} \cot(\phi/2) \\ 1 \\ -\cot 2\beta \cot(\phi/2) + \cot(\theta/2)\csc 2\beta \end{bmatrix}, \tag{5}$$

$$\alpha = \arccos\left[\frac{1}{4}(\cos 4\beta + 3)\cos\theta \cos\phi + (\sin 2\beta)^2\left(\frac{1}{2}\cos\phi - \sin^2\frac{\theta}{2}\right) + \cos 2\beta \sin\theta \sin\phi\right]. \tag{6}$$

During a searching process, the state of a quantum computer in general is

$$|\psi\rangle = (a' + bi)|1\rangle + (c + di)|2\rangle,$$

The marked state r_f

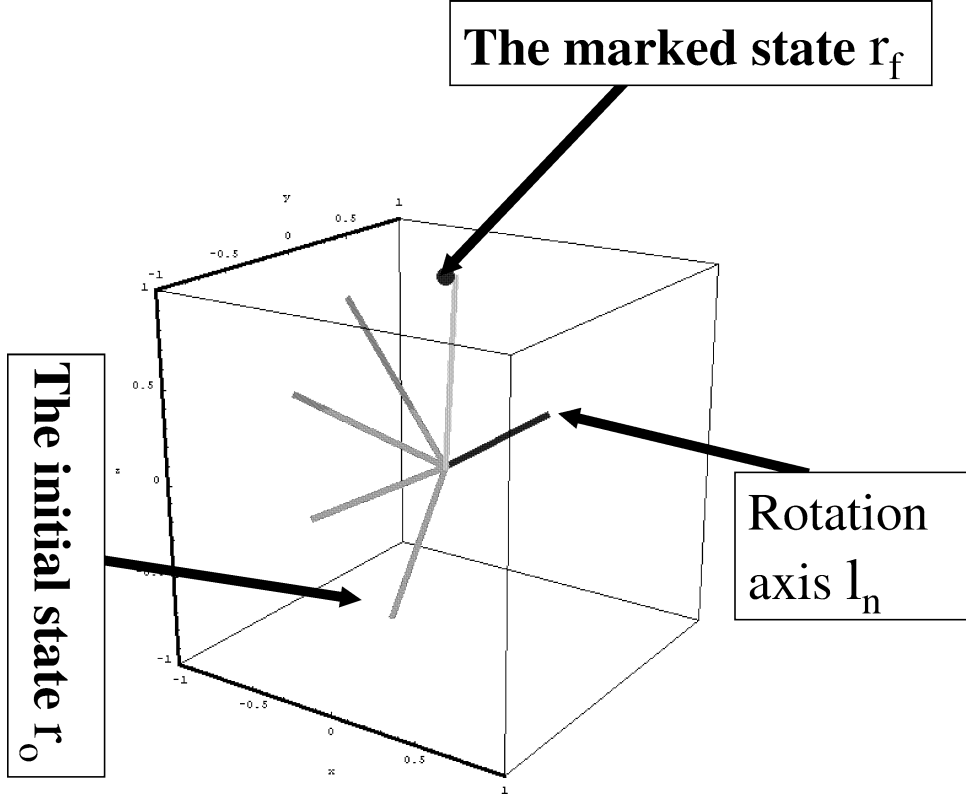**The initial state r_o**

Rotation axis l_n

Fig. 1. The rotational axis, the initial state and the marked state in the $SO(3)$ picture. The process of searching is a series of rotation of the state vector from the initial state to the marked state.

where a', b, c and d are real numbers, satisfying the normalization condition $a'^2 + b^2 + c^2 + d^2 = 1$. This state vector in the 2-dimensional space is represented by the polarization vector in the 3-dimensional space as [10]

$$\vec{r} = \langle \psi | \vec{\sigma} | \psi \rangle = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 2(a'c + bd) \\ 2(-bc + ad) \\ a'^2 + b^2 - c^2 - d^2 \end{bmatrix}, \tag{7}$$

where $\vec{\sigma}$ are the Pauli matrices. The probability of finding the marked state is

$$P = a'^2 + b^2 = (z + 1)/2. \tag{8}$$

This makes the understanding of the searching process very easy. When the state vector is the marked state, its polarization vector is $(0, 0, 1)$, and the probability according to (8) is 1. For the initial state, the polarization is about $(0, 0, -1)$ and the probability for finding the marked state is nearly zero. An illustration is given in Fig. 1.

Each searching iteration is a rotation of the polarization vector through angle α. After j iterations, the total angle rotated is

$$\omega = j\alpha,$$

and the polarization vector is rotated to

$$\vec{r}_j = \vec{r}_0 \cos \omega + \vec{l}_n (\vec{l}_n \cdot \vec{r}_0)(1 - \cos \omega) + (\vec{l}_n \otimes \vec{r}_0) \sin \omega, \tag{9}$$

where $\cdot$ and $\otimes$ are the ordinary scalar product and vector product operations. The vector $\vec{l}_n$ is the axis vector (5) normalized to unity. Using Eqs. (9) and (8), the probability for finding the marked state can be easily calculated.

During a searching process, the trajectory of the polarization vector (7) forms a cone whose rotational axis is given by (5). Starting from an initial position $\vec{r}_0$, the displacement vector $\vec{r} - \vec{r}_0$ is always perpendicular to the rotational axis. If the quantum searching process can find the marked state, then the vector $\vec{r}_f = (0, 0, 1)^\mathrm{T}$ (T means transpose) must be on the trajectory, thus $(\vec{r}_f - \vec{r}_0) \cdot \vec{l} = 0$. By putting the initial state (3) into this equation, we obtain the following phase matching condition

$$\tan\frac{\theta}{2}[\cos 2\beta + \tan\theta_0 \cos\delta \sin 2\beta] = \tan\frac{\phi}{2}\left[1 - \tan\theta_0 \sin\delta \sin 2\beta \tan\frac{\theta}{2}\right]. \tag{10}$$

This is the general phase matching condition for a successful quantum search of marked states. This phase matching condition tells us that the rotational angles depend on both the unitary transformation through β and on the initial distribution through θ_0 and δ. In previous discussions, the dependence of the phase matching condition on the initial state was ignored because the initial state was taken as $U|0\rangle = \sin\beta|1\rangle + \cos\beta|2\rangle$. In Høyer's work [12], the initial state is modified before the search, and this makes the initial state different from $U|0\rangle$, implicating the dependence on the initial state. It should be pointed out that this condition is a necessary condition for searching with certainty, but not a sufficient one. Even if this condition is met, the probability of finding marked states is not guaranteed to be 1. The standard Grover algorithm is one example. In the Grover algorithm [1], the probability of finding the marked state with optimal iterations is $\sin^2[(2j_{\mathrm{op}} + 1)\beta]$. As $\beta = \arcsin(1/\sqrt{N})$ is fixed, $(2j_{\mathrm{op}} + 1)\beta$ may not be exactly $\pi/2$.

4. Examples of phase matching conditions

It has been seen that the phase matching condition depends both on the structure of the quantum searching engine and on the initial state. Now we discuss four examples, and show that the general phase matching condition (10) is satisfied in all these cases. The differences among these four examples are in their initial states.

4.1. $|\psi_0\rangle = \sin(\theta_{\mathrm{init}})|1\rangle + \cos(\theta_{\mathrm{init}})e^{iu}|2\rangle$

In Ref. [12], although the starting state is $U|0\rangle = \sin\beta|1\rangle + \cos\beta|2\rangle$, some preparations have to be made before searching. First, the following state is obtained through 8 steps [15]:

$$|\psi_{\mathrm{init}}\rangle = \sin(\theta_{\mathrm{init}})|1\rangle + \cos(\theta_{\mathrm{init}})|2\rangle.$$

Before the searching iteration starts, a phase rotation e^{iu} is made for the unmarked state. This leaves the initial state for the quantum search engine of the form

$$|\psi_0\rangle = \sin(\theta_{\mathrm{init}})|1\rangle + \cos(\theta_{\mathrm{init}})e^{iu}|2\rangle. \tag{11}$$

In Eq. (11), $\theta_{\mathrm{init}} = \pi/2 - m\vartheta$, where $\vartheta = \arcsin|\sin(\theta/2)\sin 2\beta|$, and m is an integer:

$$m = \mathrm{INT}\left[\left(\frac{\pi}{2} - \beta\right)\Big/\vartheta\right]. \tag{12}$$

Here, INT[ ] means taking the nearest integer part.

Since θ_{init} depends numerically on the quantities involved, an analytic proof is difficult. It has been carefully checked that, by using the initial state of (11), ϕ determined by $\tan(\phi/2) = \tan(\theta/2)(1 - 2\sin^2\beta)$ fulfills the general phase matching condition (10). A numerical example is given in Appendix A.

4.2. $|\psi_0\rangle = U|0\rangle = \sin\beta|1\rangle + \cos\beta|2\rangle$

This is the initial state that the most quantum search algorithms have taken. In Ref. [7], the initial state is

$$|\psi_0\rangle = U|0\rangle = \sin\beta|1\rangle + \cos\beta|2\rangle.$$

Putting this initial state into Eq. (10) and letting $\theta_0 = \beta$ and $\delta = 0$, we obtain

$$\tan\frac{\theta}{2}(\cos 2\beta + \tan 2\beta \sin\beta) = \tan\frac{\phi}{2}.$$

Using the fact that $\cos 2\beta + \tan\beta \sin 2\beta = \cos^2\beta - \sin^2\beta + 2\sin^2\beta = 1$, we get

$$\tan\frac{\theta}{2} = \tan\frac{\phi}{2}, \quad \text{or} \quad \theta = \phi.$$

This is the result that was obtained approximately in Ref. [7], and exactly in Ref. [10] from an $SO(3)$ picture.

4.3. $|\psi_0\rangle$ used by Brassard et al. [16]

In Ref. [16], a procedure was proposed for obtaining the marked state with certainty. The strategy is to run the search algorithm $m' = m - 1$ (m is given in (12)) number of iterations with $\theta = \phi = \pi$. At this stage, the state vector of the quantum computer is just one step short of the marked state: $|\psi_0\rangle = \sin((2m'+1)\beta)|1\rangle + \cos((2m'+1)\beta)|2\rangle$. Afterwards, one does one more search with θ and ϕ determined from the following equation:

$$\cot\big\{\big(2[\tilde{m}]+1\big)\beta\big\} = e^{i\phi}\sin(2\beta)\left[-\cos(2\beta) + i\cot\frac{\theta}{2}\right]^{-1}. \tag{13}$$

We now show that the θ and ϕ determined in this way satisfy the general phase matching condition (10). Eq. (13) is equivalent to two equations, which are the real and the imaginary part, respectively:

$$\cos\phi \tan\theta_0 \sin 2\beta = -\cos 2\beta, \qquad \sin\phi \tan\theta_0 \sin 2\beta = \cot\frac{\theta}{2}.$$

Here we have introduced the notation $\theta_0 = (2m'+1)\beta$. It is then straightforward to show

$$\tan\frac{\phi}{2} = \frac{1 - \cos\phi}{\sin\phi} = \frac{1 - \frac{-\cos 2\beta}{\tan\theta_0 \sin 2\beta}}{\frac{\cot(\theta/2)}{\tan\theta_0 \sin 2\beta}} = \tan\frac{\theta}{2}[\cos 2\beta + \tan\theta_0 \sin 2\beta].$$

This is exactly the general phase matching condition (10) with $\delta = 0$. It should be pointed out that Eq. (13) is a necessary and sufficient condition for finding the marked state with certainty. It determines the two angles uniquely.

4.4. "Difficult search problem limit" of arbitrary initial distribution by Biham et al. [4]

We see from the above examples that the phase matching condition strongly depends on the initial state. Recently, using an arbitrary initial distribution, Biham et al. have studied the general quantum search algorithm with arbitrary phase rotations [4]. In particular, they obtained the phase matching condition $\theta = \phi$ which is the same as the case with $|\psi_0\rangle = U|0\rangle$. It seems contradicting that the apparent initial state dependence is missing here. The reason for this is that the phase condition of Biham et al. is obtained by using the "difficult search problem limit", $N \gg N_\tau \geqslant 1$ [4], which gives the weighted averages $|\bar{k}'(0)| = O(W_k^{-1/2})$ and $|\bar{l}'(0)| = O(1)$. This is equivalent to the case of $|\psi_0\rangle = U|0\rangle$. Thus it gives the same phase matching condition $\theta = \phi$. If this limit is not taken, then the phase matching condition can be varied greatly.

5. The computational complexity

Starting from the standard initial state $U|0\rangle$ and the standard Grover's quantum search engine, the number of iterations is $O(\sqrt{N})$. If an quasi-arbitrary initial state is used instead of the standard initial state, the number of iterations will be different from $O(\sqrt{N})$. For instance, if the initial state is just the marked state, there is no need for search at all. If the initial state is the one after m' iterations using the standard Grover as given in Ref. [16], then one needs only one iteration. Using the $SO(3)$ picture of the quantum search, it is easy to study the computational complexity of the quantum search algorithm with arbitrary phases. We give here the results, it can be proven through simple geometrical argument similar to the derivations in Ref. [17]:

(1) Given an initial state in Eq. (3) and an angle θ, determining ϕ by solving Eq. (10). (If the coefficient of the marked state is not real in the initial state, drop out a global phase factor in the initial state so that the coefficient of the marked state $|1\rangle$ is real.)

(2) Calculating the angle ω_{tot} between the initial state and the marked state in the $SO(3)$ picture by the following equation:

$$\omega_{\text{tot}} = \arccos\left(\frac{-K\sin(2\theta_0)(\cot(\phi/2)\cos\delta + \sin\delta) - \cos 2\theta_0 \csc^2(\phi/2)}{\sqrt{2K^2 + 1 + \cot^2(\phi/2) + 2K(K\cos 2\theta_0 - \sin 2\theta_0 \sin\delta - \sin 2\theta_0 \cos\delta \cot(\phi/2))}}\right), \qquad (14)$$

where

$$K = \cot\left(\frac{\theta}{2}\right)\csc(2\beta) - \cot\left(\frac{\phi}{2}\right)\cot(2\beta), \qquad (15)$$

$$\cos\alpha = \frac{1}{4}(\cos(4\beta) + 3)\cos\theta\cos\phi + \sin^2(2\beta)\left(\frac{1}{2}\cos\phi - \sin^2\left(\frac{\theta}{2}\right) + \cos 2\beta\sin\theta\sin\phi\right). \qquad (16)$$

(3) Calculating the angle α, which is the angle rotated by the quantum search engine in each iteration in the $SO(3)$ picture for given θ and the ϕ obtained through the phase matching condition.

The number of iterations required to reach maximum probability in finding the marked state is given by

$$j_{\text{op}} = \text{INT}\left[\frac{\omega_{\text{tot}}}{\alpha}\right]. \qquad (17)$$

Then maximum probability of finding the marked state is achieved by measuring the quantum computer at j_{op} or $j_{\text{op}} + 1$ step.

To find the marked state with certainty, one has to modify the above procedure a little. If one wants to construct an quantum search engine that searches the marked state with certainty near a given θ, one first uses the above procedure to obtain j_{op}. However, this quantum search engine is not guaranteed to find the marked state with certainty. One has to use slightly different angles θ and ϕ. They are determined by letting θ and ϕ as unknowns and solving the phase matching condition (10) and the equation $\omega/\alpha = J$ with $J > j_{\text{op}}$ simultaneously. Then the search algorithm with the angles so defined can find the marked state exactly when measured at Jth iteration. J can be any number equal to to greater than J_{op}. A quantum search engine for finding the marked state with certainty with the standard initial state was recently given by Long in Ref. [17].

6. Summary

We have presented a general phase matching condition with arbitrary unitary transformations and an arbitrary initial state superposed by $|1\rangle$ and $|2\rangle$. It has been shown that several phase conditions previously discussed in the literature are its special cases. Thus, there is a consistency between the results of [12] and [7] which have seemingly different expressions. The results in [16] and [4] also satisfy this general phase matching condition. The probability for obtaining the marked state has been given.

Acknowledgements

Appendix A

We give a numerical proof that the phase condition in Ref. [12] is a special case of the general phase matching condition (10). The initial state employed in Ref. [12] is

$$|\psi_0\rangle = \sin(\theta_{\text{init}})|1\rangle + \cos(\theta_{\text{init}})e^{iu}|2\rangle,$$

where $\theta_{\text{init}} = \pi/2 - m\vartheta$, $\vartheta = \sin(\theta/2)\sin(2\beta)$, $\sin\beta = \sqrt{a}$, and $m = \text{INT}[(\pi/2 - \beta)/\vartheta] + 1$. u is the difference of arguments Q_{22} and Q_{12}, and $\phi = 2\arctan[\tan(\theta/2)(1 - 2a)]$.

Taking $a = 2/400$, $\theta = \pi/2$, we have

$$\beta = \arcsin(\sqrt{a}), \qquad \vartheta = \sin\frac{\theta}{2}\sin(2\beta), \qquad m = 16, \qquad \phi = 2\arctan\left[\tan\frac{\theta}{2}(1 - 2a)\right] = 2\arctan\frac{99}{100};$$

$$Q_{11} = M_{22} = -\frac{1}{200} - \frac{199i}{200}, \qquad Q_{12} = \left(\frac{1}{200} - \frac{i}{200}\right)\sqrt{199},$$

$$Q_{21} = \left(\frac{1}{200} - \frac{i}{200}\right)\sqrt{199}e^{2i\arctan(99/100)},$$

$$u = -\left(\text{Arg}[Q_{12}] - \text{Arg}[Q_{22}]\right), \qquad \theta_{\text{init}} = \frac{\pi}{2} - m\vartheta.$$

Putting the quantities θ, ϕ, β, $\delta = u$, $\theta_0 = \theta_{\text{init}}$ into Eq. (10), we perform the calculation in *Mathematica*. With the number of digits up to 150, the result for the left side of Eq. (10) is 0.987234528 786745048 789300921 936170716 227415177 731788487 075910815 468702797 224769631 377305189 666308976 465471553 486461587 1040404 57 292323594 964054244 391216, and the one for the right-hand side is exactly the same.

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G.-L. Long et al. / Physics Letters A 294 (2002) 143–152

[15] We notice that there are some minor errors in Ref. [12], although they do not change the conclusion. (1) There is an exchange of the diagonal matrix elements in Eq. (3) of Ref. [12]; (2) We have to make a transpose to Eq. (9) in Ref. [12]; (3) During the preparation stage of the initial state in Ref. [12], step (7) should be: apply operator $Q(A, \chi, \phi, \varphi)$ a total number of m times on the first register conditionally on the third register holding a 0.

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