General SU(2) formulation for quantum searching with certainty

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(Received 7 December 2001; published 7 May 2002)

A general quantum search algorithm with arbitrary unitary transformations and an arbitrary initial state is considered in this work. To search a marked state with certainty, we have derived, using an SU(2) representation: (1) the matching condition relating the phase rotations in the algorithm, (2) a concise formula for evaluating the required number of iterations for the search, and (3) the final state after the search, with a complex phase in its amplitude. Moreover, the optimal choices and modifications of the phase angles in the Grover kernel are also studied.

DOI: 10.1103/PhysRevA.65.052322 PACS number(s): 03.67.Lx, 03.65.Ta

Quantum mechanical algorithms have recently become very popular in the field of computational science because they can speed up a computation over classical algorithms. Famous examples include the factorizing algorithm discovered by Shor [1] and the quantum search algorithm well developed by Grover [2,3]. The latter is what we intend to deal with in this work. If there is an unsorted database containing N items, and out of which only one marked item satisfies a given condition, then using Grover's algorithm one will find the object in $O(\sqrt{N})$ quantum mechanical steps instead of $O(N)$ classical steps. It has been shown that Grover's original algorithm is optimal [4–6]. But Grover's algorithm provides a high probability of finding the object only for a large N. The probability will be lower as N decreases. Grover [7], however, also proposed that the Walsh-Hadamard transformation used in the original version can be replaced by almost any arbitrary unitary operator and the phase angles of rotation can be arbitrarily used as well, instead of the original π angles. The utility of the arbitrary phase angles in fact can provide the possibility for finding the marked item with certainty, no matter whether N is large or not, if these angles obey a so-called matching condition.

Some typical literatures concerning with the matching condition will be mentioned here. Long and co-workers [8,9] have derived the relation $\phi=\theta$, where ϕ and θ are the phases used in the algorithm, using an SO(3) picture. Høyer [10], on the other hand, has proved a relation $\tan(\phi/2)=\tan(\theta/2)(1-2/N)$, and claimed that the relation $\phi=\theta$ is an approximation to this case. Recently, a more general matching condition has been derived by Long, Xiao, and Sun [11], also using the SO(3) picture. In the last article, however, only the certainty for finding the marked state is ensured. In fact, a phase angle appearing in the amplitude of the final state after searching will remain. If the final state should be necessary for a future application, i.e., if it should interact with other states, this phase angle will be important for quantum interferences, but it cannot be given in the SO(3) representation. We, therefore, intend to derive the matching condition in the SU(2) picture. Besides, we will also give a more concise formula for evaluating the number of the iterations needed in the searching and deduce the final state in a complete form as $e^{i\delta}|\tau\rangle$, where $|\tau\rangle$ is the marked state. The optimal choice of the phase angles will be discussed, too.

Suppose in a two-dimensional, complex Hilbert space we have a marked state $|\tau\rangle$ to be searched by successively operating a Grover kernel G on an arbitrary initial state $|s\rangle$. The Grover kernel is a product of two unitary operators G_τ and G_η, given by

$$G_\tau=I+(e^{i\phi}-1)|\tau\rangle\langle\tau|,$$
$$G_\eta=I+(e^{i\theta}-1)U|\eta\rangle\langle\eta|U^{-1}, \tag{1}$$

where U is an arbitrary unitary operator, $|\eta\rangle$ is another unit vector in the space, and ϕ and θ are two phase angles. It should be noted that the phases ϕ and θ actually are the differences $\phi=\phi_2-\phi_1$ and $\theta=\theta_2-\theta_1$, where ϕ_2, ϕ_1, θ_2, and θ_1, as depicted in Refs. [12,13], denote the rotating angles to $|\tau\rangle$, the vector orthogonal to $|\tau\rangle$, $U|\eta\rangle$, and the vector orthogonal to $U|\eta\rangle$, respectively. The Grover kernel can be expressed in a matrix form as long as an orthonormal set of basis vectors is designated, so we simply choose

$$|I\rangle=|\tau\rangle \quad \text{and} \quad |II\rangle=(U|\eta\rangle-U_{\tau\eta}|\tau\rangle)/l, \tag{2}$$

where $U_{\tau\eta}=\langle\tau|U|\eta\rangle$ and $l=(1-|U_{\tau\eta}|^2)^{1/2}$. Letting $U_{\tau\eta}=\sin(\beta)e^{i\alpha}$, we can write, from Eq. (2),

$$U|\eta\rangle=\sin(\beta)e^{i\alpha}|I\rangle+\cos(\beta)|II\rangle, \tag{3}$$

and the Grover kernel can now be written as

$$G=-G_\eta G_\tau=-\begin{bmatrix} e^{i\phi}[1+(e^{i\theta}-1)\sin^2(\beta)] & (e^{i\theta}-1)\sin(\beta)\cos(\beta)e^{i\alpha} \\ e^{i\phi}(e^{i\theta}-1)\sin(\beta)\cos(\beta)e^{-i\alpha} & 1+(e^{i\theta}-1)\cos^2(\beta) \end{bmatrix}. \tag{4}$$

In the searching process, the Grover kernel is successively operated on the initial state $|s\rangle$. We wish that after, say, m iterations the operation the final state will be orthogonal to the basis vector $|II\rangle$ so that the probability for finding the marked state $|\tau\rangle$ will exactly be unity. Alternatively, in mathematical expression, we wish to fulfill the requirement

$$\langle II|G^m|s\rangle = 0, \tag{5}$$

since then

$$|\langle \tau|G^m|s\rangle| = |\langle I|G^m|s\rangle| = 1. \tag{6}$$

The eigenvalues of the Grover kernel G are

$$\lambda_{1,2} = -\exp\left[i\left(\frac{\phi+\theta}{2} \pm w\right)\right], \tag{7}$$

where the angle w is defined by

$$\cos(w) = \cos\left(\frac{\phi-\theta}{2}\right) - 2\sin\left(\frac{\phi}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin^2(\beta). \tag{8}$$

The normalized eigenvectors associated with these eigenvalues are computed:

$$|g_1\rangle = \begin{bmatrix} e^{-i(\phi/2)}e^{i\alpha}\cos(x) \\ \sin(x) \end{bmatrix}, \quad |g_2\rangle = \begin{bmatrix} -\sin(x) \\ e^{i(\phi/2)}e^{-i\alpha}\cos(x) \end{bmatrix}. \tag{9}$$

In expression (9), the angle x is defined by

$$\sin(x) = \sin\left(\frac{\theta}{2}\right)\sin(2\beta)/\sqrt{l_m},$$

where

$$l_m = \left[\sin(w) + \sin\left(\frac{\phi-\theta}{2}\right) + 2\cos\left(\frac{\phi}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin^2(\beta)\right]^2 + \left[\sin\left(\frac{\theta}{2}\right)\sin(2\beta)\right]^2 = 2\sin(w)\left[\sin(w) + \sin\left(\frac{\phi-\theta}{2}\right) + 2\cos\left(\frac{\phi}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin^2(\beta)\right].$$

The matrix G^m can be simply expressed by $G^m = \lambda_1^m|g_1\rangle\langle g_1| + \lambda_2^m|g_2\rangle\langle g_2|$, so we have

$$G^m = (-1)^m e^{im[(\phi+\theta)/2]}\begin{bmatrix} e^{imw}\cos^2(x) + e^{-imw}\sin^2(x) & e^{-i(\phi/2)}e^{i\alpha}i\sin(mw)\sin(2x) \\ e^{i(\phi/2)}e^{-i\alpha}i\sin(mw)\sin(2x) & e^{imw}\sin^2(x) + e^{-imw}\cos^2(x) \end{bmatrix}. \tag{10}$$

The initial state $|s\rangle$ in this work is considered to be an arbitrary unit vector in the space and is given by

$$|s\rangle = \sin(\beta_0)|I\rangle + \cos(\beta_0)e^{iu}|II\rangle. \tag{11}$$

The requirement (5) implies that both the real and imaginary parts of the term $\langle II|G^m|s\rangle$ are zero, so, as substituting Eqs. (10) and (11) into Eq. (5), one will eventually obtain the two equations

$$-\sin(mw)\sin\left(\frac{\phi}{2} - \alpha - u\right)\sin(2x)\sin(\beta_0) + \cos(mw)\cos(\beta_0) = 0, \tag{12}$$

$$\sin(mw)\cos\left(\frac{\phi}{2} - \alpha - u\right)\sin(2x)\sin(\beta_0) - \sin(mw)\cos(2x)\cos(\beta_0) = 0. \tag{13}$$

Equation (13), by the definition of the angle x, will reduce to the matching condition

$$\left[\sin\left(\frac{\phi-\theta}{2}\right) + 2\cos\left(\frac{\phi}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin^2(\beta)\right]\cos(\beta_0) = \sin\left(\frac{\theta}{2}\right)\sin(2\beta)\cos\left(\frac{\phi}{2} - \alpha - u\right)\sin(\beta_0), \tag{14}$$

which is identical to the relation derived by Long, Xiao, and Sun [11],

$$\tan\left(\frac{\phi}{2}\right) = \tan\left(\frac{\theta}{2}\right)\left(\frac{\cos(2\beta) + \sin(2\beta)\tan(\beta_0)\cos(\alpha+u)}{1 - \tan(\beta_0)\tan\left(\frac{\theta}{2}\right)\sin(2\beta)\sin(\alpha+u)}\right). \tag{15}$$

Equation (12), under the satisfaction of the matching condition (14), or (15), will reduce to a concise formula for evaluating the number of iterations m,

$$\cos\left\{mw + \sin^{-1}\left[\sin(\beta_0)\sin\left(\frac{\phi}{2} - \alpha - u\right)\right]\right\} = 0. \tag{16}$$

By Eq. (16), one can compute the number m,

$$m = \lceil f \rceil, \tag{17}$$

where $\lceil\,\rceil$ denotes the smallest integer greater than the quantity in it, and the function f is given by

$$f = \frac{\frac{\pi}{2} - \sin^{-1}\left[\sin(\beta_0)\sin\left(\frac{\phi}{2} - \alpha - u\right)\right]}{\cos^{-1}\left[\cos\left(\frac{\phi-\theta}{2}\right) - 2\sin\left(\frac{\phi}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin^2(\beta)\right]}. \tag{18}$$

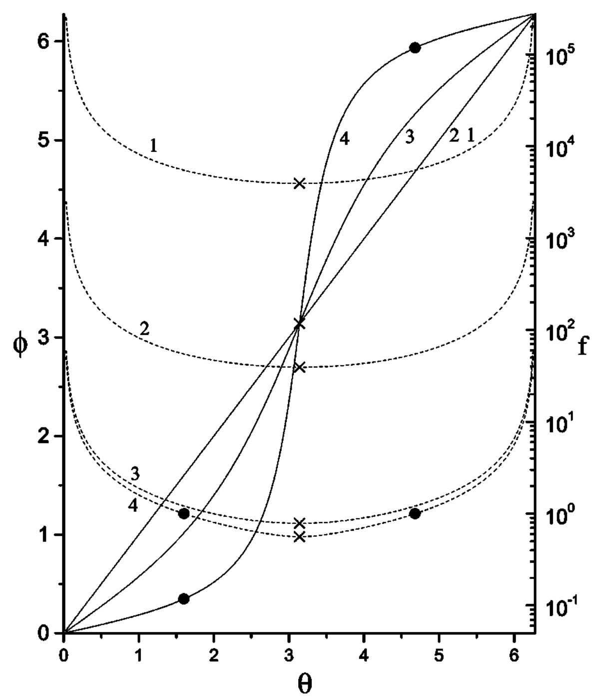

FIG. 1. Variations of $\phi(\theta)$ (solid) and $f(\theta)$ (broken), for $\alpha+u=0$, $\beta_0=10^{-4}$, and $\beta=10^{-4}$ (1), 10^{-2} (2), 0.5 (3), and 0.7 (4), respectively. The crosses denote the special case of Høyer [10], while the full circles correspond to the optimal choices of $\phi_{\rm op}$ and $\theta_{\rm op}$ for $\alpha+u=0$, $\beta_0=10^{-4}$, and $\beta=0.7$. The solid straight line 1 corresponds to the case $\phi=\theta$, while the solid curve 2 is only approximately close to the former.

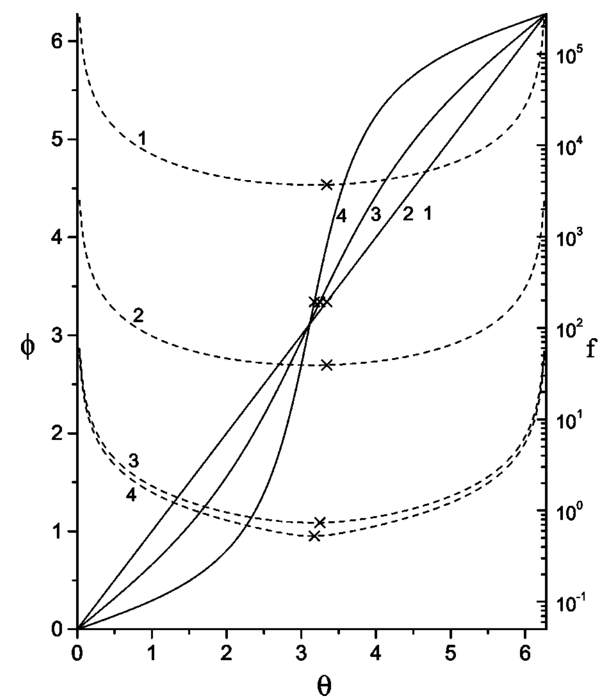

FIG. 2. Variations of $\phi(\theta)$ (solid) and $f(\theta)$ (broken), for $\alpha+u=0.1$, $\beta_0=0.1$, and $\beta=10^{-4}$ (1), 10^{-2} (2), 0.5 (3), and 0.7 (4), respectively. The crosses denote the special case of Høyer [10]. The solid curves 1 and 2 are very close, and both of them are only approximately close to the line $\phi=\theta$.

It can also be shown that if the matching condition is fulfilled, then after m searching iterations the final state will be

$$G^m|s\rangle=e^{i\delta}|\tau\rangle=\exp\left\{i\left[m\left(\pi+\frac{\phi+\theta}{2}\right)+\Omega\right]\right\}|\tau\rangle, \quad (19)$$

where the angle Ω is defined by

$$\Omega=\tan^{-1}\left[\cot\left(\frac{\phi}{2}-\alpha-u\right)\right]. \quad (20)$$

The phase angle appearing in the amplitude of the final state will be important for quantum interferences if possibly the state should interact with other states in a future application, so we would better had it remain in the present form.

The matching condition (14), or (15), relates the angles ϕ, θ, β, β_0, and $\alpha+u$ for finding a marked state with certainty. If β, β_0, and $\alpha+u$ are designated, then $\phi=\phi(\theta)$ is deduced by the matching condition. As $\phi(\theta)$ is determined, we then can evaluate by Eq. (18) the value of $f=f(\phi(\theta),\theta)$ and consequently decide by Eq. (17) the number of iterations m. The functions $\phi(\theta)$ and $f(\theta)$ for some particular designations of β, β_0, and $\alpha+u$ have been shown in Figs. 1 and 2. These examples have schematically depicted that theoretically we can establish a tabulated chart of possible choices between all of the phases for finding a marked state with certainty. It is worth noticing that as $\alpha+u=0$ and $\beta=\beta_0$, the matching condition recovers $\phi=\theta$ automatically since then Eq. (13) becomes an identity, and accordingly one has

$$f=\frac{\dfrac{\pi}{2}-\sin^{-1}\left[\sin\left(\dfrac{\phi}{2}\right)\sin(\beta)\right]}{2\sin^{-1}\left[\sin\left(\dfrac{\phi}{2}\right)\sin(\beta)\right]} \quad \text{for} \quad \phi=\theta. \quad (21)$$

This is the case discussed in Ref. [9]; an example can be read by the straight line of unity slope for $\beta=\beta_0=10^{-4}$ and the corresponding f vs θ variation in Fig. 1. It can also be shown that the matching condition (14) will recover the relation considered by Høyer [10],

$$\tan\left(\frac{\phi}{2}\right)=\tan\left(\frac{\phi}{2}\right)\cos(2\beta) \quad \text{for} \quad \cos(\phi/2-\alpha-u)=0. \quad (22)$$

In Figs. 1 and 2 we have shown by the cross marks some particular examples of this special case.

Observing Figs. 1 and 2, one realizes that for every designation of β, β_0, and $\alpha+u$, the optimal choices for ϕ and θ is letting $\phi=\theta=\pi$, since then the corresponding f is minimum under the fact $df/d\theta=(\partial f/\partial\phi)(d\phi/d\theta)+\partial f/\partial\theta=0$, for $\phi=\theta=\pi$. We thus denote the optimal value of m by

$$m_{\rm op}=\lceil\min(f)\rceil=\left\lceil\frac{\dfrac{\pi}{2}-\sin^{-1}[\sin(\beta_0)\cos(\alpha+u)]}{2\beta}\right\rceil. \quad (23)$$

With the choice of m_{op}, however, one needs to modify the phases θ and $\phi(\theta)$ to depart from π so that the matching condition is satisfied again. For example, if $\alpha+u=0$, $\beta_0=10^{-4}$, and $\beta=0.7$ are designated, then the minimum value of f will be $\min(f)=0.56$. So we choose $m_{\mathrm{op}}=1$ and the modified phases are $\theta_{\mathrm{op}}=(1\pm 0.490)\pi$ and $\phi_{\mathrm{op}}=(1\pm 0.889)\pi$, respectively. This example has been shown by the marked entire circles in Fig. 1. It is worth noticing again that under the choice of m_{op} the modified ϕ and θ for the special case considered by Long [9] will be

$$\phi_{\mathrm{op}}=\theta_{\mathrm{op}}=2\sin^{-1}\left(\frac{\sin\left(\frac{\pi}{4m_{\mathrm{op}}+2}\right)}{\sin(\beta)}\right),$$

where

$$m_{\mathrm{op}}=\left\lceil\frac{\frac{\pi}{2}-\beta}{2\beta}\right\rceil.$$

This is in fact a special case in which the phases ϕ_{op} and θ_{op} can be given by a closed-form formula.

To summarize, using the SU(2) representation we have derived the matching condition (14) for finding with certainty a marked state with arbitrary unitary transformations and an arbitrary initial state. The formula (17), together with Eq. (18), has also been deduced for evaluating the required number of iterations for the search. Moreover, the final state with a phase angle in its amplitude, which cannot be given by the SO(3) picture used in Ref. [11], has been consequently obtained. The optimal choice $\phi=\theta=\pi$ under any designation of β, β_0, and $\alpha+u$ has been shown. However, for finding the marked state with certainty, the phases ϕ and θ need to be modified since m_{op} must be an integer. An example to depict the modification of ϕ and θ, therefore, has also been given.

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