More General Quantum Search Algorithm $Q = -I_\gamma VI_\tau U$

And the Precise Formula for the Amplitude and
the Non-symmetric Effects of Different Rotating Angles

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Abstract

This paper presented two general quantum search algorithms. We derived the iterated formulas and the simpler approximate formulas and the precise formula for the amplitude in the desired state. A mathematical proof of Grover’s algorithm being optimal among the algorithms with arbitrary phase rotations was given in this paper. This first reported the non-symmetric effects of different rotating angles, and gave the first-order approximate phase condition when rotating angles are different.

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1 Introduction

Shor reported his prime factoring algorithm in [5]. Then Grover gave his quantum search algorithm [2][3]. In [2] Grover’s quantum search algorithm consists of a sequence of unitary operations on a pure state. The algorithm is $Q = -I_0^{(\pi)}WI_\tau^{(\pi)}W$, where $I_0^{(\pi)} = I - 2|\langle x | \rangle| | x \rangle$ and inverts the amplitude in the state $| x \rangle$, $W$ is Walsh-Hadamard transformation. It would carry out repeated operations of $Q$, that is, $...(-I_0^{(\pi)}WI_\tau^{(\pi)}W)(-I_0^{(\pi)}WI_\tau^{(\pi)}W)(-I_0^{(\pi)}WI_\tau^{(\pi)}W)...$

$= ...(-WI_0^{(\pi)}W)I_0^{(\pi)}(-WI_0^{(\pi)}W)I_0^{(\pi)}(-WI_0^{(\pi)}W)I_0^{(\pi)}...$, where $(-WI_0^{(\pi)}W)$ is just the inversion-about-average operation. Therefore Grover’s algorithm consists of alternating iteration of $(-WI_0^{(\pi)}W)$, 

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inversion about the average, and \( I_\gamma^{(\pi)} \), inversion of the amplitude in the desired state \(| \gamma \rangle \). Then in \([2]\) Grover showed how to replace Walsh-Hadamard transformation in his original algorithm with an arbitrary quantum mechanical operation, obtained the quantum search algorithm \( Q = -I_\gamma^{(\pi)} U^{-1} I_\tau^{(\pi)} U \), where \( U \) is an arbitrary unitary operation and \( U^{-1} \) is the adjoint (the complex conjugate of the transpose) of \( U \). Grover thinks that it leads to several new applications and broadens the scope for implementation. When the amplitudes are rotated by arbitrary phases, instead of being inverted, that is, \( Q = -I_\gamma^{(\theta)} U^{-1} I_\tau^{(\phi)} U \), where \( I_\gamma^{(\theta)} = I - (e^{i\theta} + 1)|x\rangle\langle x| \), Long et al. first found that \( \theta \) and \( \phi \) must satisfy a matching condition: \( \theta = \phi \), and derived an approximate formula for the amplitude in the amplitude amplification \([1]\) and studied the effects of using arbitrary phases in amplitude amplification \([3]\). In \([4]\) the phase condition that \( \tan(\phi/2) = \tan(\phi/2)(1 - a) \) was presented. In \([5]\) the recursion equations were used to study the quantum search algorithm.

Here, this paper presented two general quantum search algorithms, derived the iterated formulas and the simpler approximate formulas of the amplitudes in the desired state. We showed that the amplitude in the desired state can be precisely written as a polynomial in \( (\beta \lambda) \) for any quantum search algorithms which preserve a two-dimensional vector space. This is the first precise formula of the amplitude amplification in the desired state for the general quantum search algorithms including Grover’s and Long et al.’ and Hoyer’s ones. The precise formula for the amplitude can help derive a precise phase condition. A mathematical proof was given in this paper for that Grover’s algorithm is optimal among the quantum search algorithms with arbitrary phase rotations. We first found that the effects of rotating angles in the initial state and the desired state on the amplitude of the desired state are not symmetric. We also discussed the amplitude amplifications, and gave the first-order approximate phase condition when rotating angles are different.

2 More general quantum search algorithm \( Q = -I_\gamma V I_\tau U \)

Let \( I_\gamma^{(\theta)} = I - (e^{i\theta} + 1)|x\rangle\langle x| \). Grover studied the quantum search algorithm in \([3]\): \( Q = -I_\gamma^{(\pi)} U^{-1} I_\tau^{(\pi)} U \), where \( U \) is an arbitrary unitary operator and \( U^{-1} \) is the adjoint (the complex conjugate of the transpose) of \( U \) and \( I_\tau^{(\pi)} \) inverts the amplitude in the state \(| x \rangle \). Generally let \( I_x = I - a e^{i\theta}|x\rangle\langle x| \). Then \( I_x \) is unitary if and only if \((1 - ae^{i\theta})(1 - ae^{-i\theta}) = 1 \). That is, \( a = 2 \cos \theta \).

Then \( I_x = I - 2 \cos \theta e^{i\theta}|x\rangle\langle x| \) when \( \theta = 0 \), \( I_x = I_\gamma^{(\pi)} \). If let \( I_x' = I - (ae^{i\theta} + 1)|x\rangle\langle x| \), then \( I_x' \) is unitary if and only if \( a = \pm 1 \). That is, \( I_x' = I_\gamma^{(\theta)} \) or \( I_x^{(\pi+\theta)} \). Clearly \( I_x^{(\pi+\theta)} = I_x^{(\pi)} I_\gamma^{(\theta)} \) and \( I_x^{(\pi+\theta)} = I - 2 \cos \theta e^{i\theta}|x\rangle\langle x| \) and \( I_x = I - 2 \cos \theta e^{i\theta}|x\rangle\langle x| = I_x^{(\pi+\theta)} I_\gamma^{(\theta)} = I_x^{(\pi)} (I_\gamma^{(\theta)})^2 \). Long et
al. studied the phase matching condition for the algorithm $Q = -I_\gamma^{(1)} U^{-1} I_\gamma^{(\phi)} U$.

Let’s study the quantum search algorithm $Q = -I_\gamma V I_\gamma U$, where $V$ and $U$ are arbitrary unitary $N \times N$ matrices, where $N = 2^n$ for $n$ qubits, and $I_\gamma = I - 2 \cos \theta e^{i\theta} |\gamma\rangle \langle \gamma|$ and $I_\tau = I - 2 \cos \phi e^{i\phi} |\tau\rangle \langle \tau|$.  

Since $V$ and $U$ are unitary, $(VU)$ is also unitary, where $(VU)$ is the product of $V$ by $U$. Then by the definition $(VU)^{-1} = (VU)^+$ which is the adjoint (the complex conjugate of the transpose) of $(VU)$. Assume that $(VU)$ is hermitian. By the definition $(VU) = (VU)^+$, therefore $(VU)(VU) = (VUVU) = I$, where $(VUVU)$ is the product of the matrices. In fact, given that $(VU)$ is unitary then $(VU)$ is hermitian if and only if $(VUVU) = I$. We give a proof as follows. Since $(VU)$ is unitary and hermitian, $(VU)(VU) = (VU)(VU)^+ = I$. Conversely, from that $(VUVU) = I$, we obtain $(VU)(VU)(VU)^+ = UVUVU)$ since $V$ is unitary, then $(VU) = (VU)^+$. Therefore by the definition $VU$ is hermitian.

For Grover’s algorithm $V = U^{-1}$ clearly $(VU)$ is hermitian. Here we give a sufficient condition in which $(VU)$ is hermitian as follows. If $V$ and $U$ are hermitian and $V$ and $U$ are commutative, then $(VU)$ is hermitian since by the definition $V = V^+$ and $U = U^+$ and $(VU)^+ = U^+ V^+ = UV = VU$.

On the assumption that $(VU)$ is hermitian we will show that $Q$ preserves the four-dimensional vector space spanned by $|\gamma\rangle$, $(VU)|\gamma\rangle$, $V|\tau\rangle$ and $U^{-1}|\tau\rangle$. After obtain $V|\tau\rangle$ and $U^{-1}|\tau\rangle$, we apply $V^{-1}$ to $V|\tau\rangle$ or $U$ to $U^{-1}|\tau\rangle$, then obtain the desired state $|\tau\rangle$. Let’s calculate the amplitude in the desired state $V|\tau\rangle$ and $U^{-1}|\tau\rangle$. We will use the notations in $\mathcal{H}$, $\langle \tau|U|\gamma\rangle = U_{\tau\gamma}$, $\langle \gamma|V|\tau\rangle = V_{\gamma\tau}$, $\langle \tau|V^{-1}|\gamma\rangle = V_{\tau\gamma}^*$, $\langle \tau|(UV)|\tau\rangle = (UV)_{\tau\tau}$, $\langle \gamma|(VU)|\gamma\rangle = (VU)_{\gamma\gamma}$. After calculating $Q|\gamma\rangle$, $Q((VU)|\gamma\rangle)$, $Q(V|\tau\rangle)$ and $Q(U^{-1}|\tau\rangle)$ we obtain the following express.

$$Q = \begin{pmatrix}
|\gamma\rangle \\
(VU)|\gamma\rangle \\
V|\tau\rangle \\
U^{-1}|\tau\rangle
\end{pmatrix} = M \begin{pmatrix}
|\gamma\rangle \\
(VU)|\gamma\rangle \\
V|\tau\rangle \\
U^{-1}|\tau\rangle
\end{pmatrix},$$

where

$$M = \begin{pmatrix}
2 \cos \theta e^{i\theta} ((VU)_{\gamma\gamma} - 2 \cos \phi e^{i\phi} U_{\gamma\tau} V_{\tau\gamma}) & -1 & 2 \cos \phi e^{i\phi} U_{\gamma\tau} & 0 \\
-1 + 2 \cos \theta e^{i\theta} - 4 \cos \theta e^{i\theta} \cos \phi e^{i\phi} |V_{\gamma\tau}|^2 & 0 & 2 \cos \phi e^{i\phi} V_{\gamma\tau}^* & 0 \\
2 \cos \theta e^{i\theta} U_{\gamma\tau}^* - 4 \cos \theta e^{i\theta} \cos \phi e^{i\phi} V_{\gamma\tau}^* (UV)_{\tau\tau} & 0 & 2 \cos \phi e^{i\phi} (UV)_{\tau\tau} & -1 \\
2 \cos \theta e^{i\theta} (1 - 2 \cos \phi e^{i\phi}) V_{\gamma\tau} & 0 & 2 \cos \phi e^{i\phi} - 1 & 0
\end{pmatrix}.$$}

2.1 The iterated formula for the amplitude

Next we derive the iterated formula for the amplitudes in the states $|\gamma\rangle$, $(VU)|\gamma\rangle$, $V|\tau\rangle$ and $U^{-1}|\tau\rangle$ for $Q^k|\gamma\rangle$ after $k$ operations of $Q$. 

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Let $Q|\gamma\rangle = l_1|\gamma\rangle - (VU)|\gamma\rangle + p_1(V|\tau\rangle)$,

$Q((VU)|\gamma\rangle) = l_2|\gamma\rangle + p_2(V|\tau\rangle)$,

$Q(V|\tau\rangle) = l_3|\gamma\rangle + p_3(V|\tau\rangle) - U^{-1}|\tau\rangle$,

$Q(U^{-1}|\tau\rangle) = l_4|\gamma\rangle + p_4(V|\tau\rangle)$.

Let $Q^k|\gamma\rangle = a_k|\gamma\rangle + b_k((VU)|\gamma\rangle) + c_k(V|\tau\rangle) + d_k(U^{-1}|\tau\rangle)$, where $a_k, b_k, c_k$ and $d_k$ are the amplitudes in the states $|\gamma\rangle$, $((VU)|\gamma\rangle)$, $(V|\tau\rangle)$ and $(U^{-1}|\tau\rangle)$, respectively. Then $Q^{k+1}|\gamma\rangle = Q(Q^k|\gamma\rangle) = a_kQ|\gamma\rangle + b_kQ((VU)|\gamma\rangle) + c_kQ(V|\tau\rangle) + d_kQ(U^{-1}|\tau\rangle)$. Then we obtain the following iterated formula: $a_{k+1} = l_1a_k + l_2b_k + l_3c_k + l_4d_k$, $b_{k+1} = -a_k$, $c_{k+1} = p_1a_k + p_2b_k + p_3c_k + p_4d_k$, $d_{k+1} = -c_k$.

### 2.2 The first-order approximate formula for the amplitude

From the iterated formula we will approximate $c_{k+1}$ using the first-order Taylor formula of $U_{\tau\gamma}$. That is, in $c_{k+1}$ we only keep the first-order of $U_{\tau\gamma}$ and omit the high order of $U_{\tau\gamma}$. Let $V_{\tau\tau} = U^*_{\tau\gamma}$, $(VU)_{\gamma\gamma} = (UV)_{\tau\tau} = 0$ to approximate $c_{k+1}$. Let’s give a brief justification as follows. Clearly if $V = \pm U^{-1}$, then $(VU) = \pm I$, then $(VU)_{\gamma\gamma} = (UV)_{\tau\tau} = \pm 1$. Therefore assume that $V \neq \pm U^{-1}$. Let $w_{ij}$ be any term of a unitary matrix $W$. Then by the definition $WW^+ = W^+W = I[I]$. $\sum_k w_{ki}\bar{w}_{kj} = \sum_k w_{ik}\bar{w}_{jk} = \delta_{ij}$, where $\delta_{ij}$ is the Kronecker delta and $\bar{w}_{kj}$ is the complex conjugate of $w_{kj}$. That is, each row(column) of $W$ has length one and any two rows(columns) of $W$ are orthogonal. Clearly $|w_{ij}| \leq 1$. If $|w_{ij}| = 1$, then all terms of the $i$th row and the $j$th column of $W$ are zero except the $ij$ term. The results above hold for $V, U, (VU)$ and $(UV)$ since they are unitary. Specially $|(VU)_{\gamma\gamma}| \leq 1$ and $|(UV)_{\tau\tau}| \leq 1$.

If $W$ is assumed to be hermitian $[I]$, then by the definition $W = W^+$, that is, $w_{ij} = \bar{w}_{ji}$, then all the diagonal terms $ii$ of $W$ are real. Since $V$ is unitary and $(VU)$ is assumed to be hermitian, it is easy to show that $(UV)$ also is hermitian. By the definition $(VU) = (UV)^+ = U^+V^+$, then $V^+(VU)V = V^+(U^+V^+)V$, $UV = V^+U^+ = (UV)^+$, therefore $(UV)$ also is hermitian. So all the diagonal terms of $(VU)$ and $(UV)$ are real. Specially $(VU)_{\gamma\gamma}$ and $(UV)_{\tau\tau}$ are real.

Next we will give a sufficient condition in which all the diagonal terms of $(VU)$ and $(UV)$ are zero. For the detail please see the appendix 4.

If $V$ is unitary and each $V_{ij}$ of the block form of $V$ is of the form $\begin{pmatrix} a & b \\ b & a \end{pmatrix}$, and $U = V^+P$. Then $U$ is unitary, $(VU)$ and $(UV)$ are unitary and hermitian, and all the diagonal terms of $(VU)$ and $(UV)$ are zero. For the definition of $P$ please see the appendix 4.

Now let us make the first-order approximate formula for the amplitude. Since $p_1$ and $p_2$
contain the factor $U_{\tau\gamma}$, we have to approximate $a_k$ with the expression without $U_{\tau\gamma}$. From $Q|\gamma\rangle$ and $Q^2|\gamma\rangle$ $a_1 = 0, b_1 = -1, c_1 = 2\cos\phi e^{i\phi}U_{\tau\gamma}, d_1 = 0; a_2 = -e^{i2\theta}, b_2 = 0, c_2 = -2\cos\phi e^{i\phi}U_{\tau\gamma}, d_2 = -2\cos\phi e^{i\phi}U_{\tau\gamma}$. By induction we obtain $a_{k+1} = -e^{i2\theta}a_{k-1}, a_k = \begin{cases} 0, & k \text{ is odd;} \\ (-1)^m e^{i2m\theta}, & k = 2m. \end{cases}$

$$c_{k+1} = 2\cos\phi e^{i\phi}(a_k-a_{k-1})U_{\tau\gamma} + (1-2\cos\phi e^{i\phi})c_k-1, c_{k+1} = \begin{cases} (-1)^m 2\cos\phi e^{i\phi}U_{\tau\gamma} \sum_{l=0}^{m} \sigma^{(m-l)}\delta^l, & k = 2m; \\ (-1)^m 2\cos\phi e^{i\phi}U_{\tau\gamma} \sum_{l=0}^{m} \sigma^{(m-l)}\delta^l, & k = 2m+1; \end{cases}$$

where $\sigma = 2\cos\theta e^{i\theta} - 1 = e^{i2\theta}, \delta = 2\cos\phi e^{i\phi} - 1 = e^{i2\phi}$.

Case 1, $\sigma = \delta$. That is, $\theta = \phi$, which is called phase matching condition by Long et al.’s terminology.

In the case $c_{k+1} = \begin{cases} (-1)^m (k+2) \cos\phi e^{i\phi} e^{i\phi} U_{\tau\gamma}, & k = 2m; \\ (-1)^{m+1} (k+1) \cos\phi e^{i\phi} e^{i\phi} U_{\tau\gamma}, & k = 2m+1; \end{cases}$

$|c_{k+1}| = \begin{cases} (k+2) |\cos\phi| U_{\tau\gamma}|, & k = 2m; \\ (k+1) |\cos\phi| U_{\tau\gamma}|, & k = 2m+1. \end{cases}$

Therefore for arbitrary unitary operators $V$ and $U$, when $(VU)$ is hermitian, $Q = -I_{\gamma}VI_{\tau\gamma}U$ can be used to construct a quantum search algorithm that succeeds with certainty except that $I_{\gamma} = I$ or $I_{\tau} = I$. The number of iterations is almost $1/|\cos\phi| U_{\tau\gamma}|$ to reach the desired state $|\tau\rangle$ from the initial state $|\gamma\rangle$.

Specially when $\sigma = \delta = 1$, that is, $\theta = \phi = 0$, then $I_{\gamma} = I^{(\pi)}_{\gamma}, I_{\tau} = I^{(\pi)}_{\tau}$, the algorithm becomes $-I^{(\pi)}_{\gamma} V I^{(\pi)}_{\tau} U$, and

$$Q \begin{pmatrix} |\gamma\rangle \\ (VU)|\gamma\rangle \\ V|\tau\rangle \\ U^{-1}|\tau\rangle \end{pmatrix} = \begin{pmatrix} (2(VU)_{\gamma\gamma} - 4U_{\tau\gamma}V_{\gamma\tau}) & -1 & 2U_{\tau\gamma} & 0 \\ (1-4|V_{\tau\gamma}|^2) & 0 & 2V^*_{\tau\gamma} & 0 \\ (2U_{\gamma\tau} - 4V_{\tau\gamma}(VU)_{\tau\tau}) & 0 & 2(UV)_{\tau\tau} & -1 \\ -2V_{\tau\gamma} & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} |\gamma\rangle \\ (VU)|\gamma\rangle \\ V|\tau\rangle \\ U^{-1}|\tau\rangle \end{pmatrix}.$$
3 The precise formula for the amplitude for the general algorithms which preserve a two-dimensional vector space and the non-symmetric effects of different rotating angles

Though in the algorithm $Q = -I_\gamma V I_\tau U$ in the section 1 above let $V = U^{-1}$ then obtain the algorithm in this section $Q = -I_\gamma U^{-1} I_\tau U$, note that in the section 1 when we derived the iterated and approximate formulas of the amplitudes in the state $V|\tau\rangle$ we assumed $V_{\gamma\tau} = U_{\gamma\tau}^*$, $(VU)_{\gamma\gamma} = (UV)_{\tau\tau} = 0$. And in the section 1 $Q$ preserves the four-dimensional vector space spanned by $|\gamma\rangle, (VU)|\gamma\rangle, V|\tau\rangle$ and $U^{-1}|\tau\rangle$. In this section we will show that $Q$ preserves the two-dimensional vector space spanned by $|\gamma\rangle$ and $U^{-1}|\tau\rangle$, clearly $V_{\gamma\tau}, (VU)_{\gamma\gamma}$ and $(UV)_{\tau\tau}$ don’t appear. So the results in this section can not be obtained from the ones in the section 1 by simply letting $V = U^{-1}$. So for the algorithm in this section it is necessary to derive its iterated formula, precise one and approximate one of the amplitude in the desired state and discuss its amplitude amplification.

Let’s study the algorithm $Q = -I_\gamma U^{-1} I_\tau U$, where $I_\gamma = I - 2\cos\theta e^{i\phi}|\gamma\rangle\langle\gamma|$ and $I_\tau = I - 2\cos\theta e^{i\phi}|\tau\rangle\langle\tau|$. When $\theta = \phi = 0$, it reduces to Grover’s algorithm.

After calculating, we obtain the following expression. For detailed derivation, please see the appendix 3.

$$Q \begin{pmatrix} |\gamma\rangle \\ U^{-1}|\tau\rangle \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \lambda & \delta \end{pmatrix} \begin{pmatrix} |\gamma\rangle \\ U^{-1}|\tau\rangle \end{pmatrix}$$

where $\alpha = -\{1 - 2\cos\theta e^{i\phi} + 4\cos\theta e^{i\phi}\cos\phi e^{i\phi}|U_{\gamma\tau}|^2\}, \beta = 2\cos\phi e^{i\phi}U_{\gamma\tau}, \lambda = 2\cos\theta e^{i\phi}(1 - 2\cos\phi e^{i\phi})U_{\gamma\tau}, \delta = 2\cos\phi e^{i\phi} - 1$. Clearly the present algorithm $Q$ like Grover’s and Long et al.’s algorithms preserves the vector space spanned by $|\gamma\rangle$ and $U^{-1}|\tau\rangle$.

For Grover’s algorithm $\alpha = 1 - 4|U_{\tau\gamma}|^2, \beta = 2U_{\tau\gamma}, \lambda = -2U_{\tau\gamma}, \delta = 1$.

For Long et al.’s algorithm $\alpha = -e^{i\theta} - (e^{i\theta} + 1)(e^{i\phi} + 1)|U_{\gamma\tau}|^2, \beta = (e^{i\phi} + 1)U_{\gamma\tau}, \lambda = (-e^{i\theta} + 1)e^{i\phi}U_{\tau\gamma}, \delta = -e^{i\phi}$.

Hoyer’s algorithm preserves a two-dimensional vector space spanned by another two states, where $\alpha = -\{(1 - e^{i\phi})a + e^{i\phi}\}, \beta = (1 - e^{i\phi})\sqrt{a}\sqrt{1 - a}e^{i\phi}, \lambda = (1 - e^{i\phi})\sqrt{a}\sqrt{1 - a}, \delta = \{(1 - e^{i\phi})a - 1\}e^{i\phi}$.

The process of deriving the following iterated formula and precise formula for the amplitude is the same for the present algorithm and Grover’ and Long et al.’s and Hoyer’s algorithms and any other quantum search algorithms which preserve a two-dimensional vector space, this is because the derivation is not concerned in the contents of $\alpha, \beta, \lambda$ and $\delta$. 

6
3.1 The iterated formula for the amplitude

Let’s derive the iterated formula for the amplitude in the desired state $U^{-1}|\tau\rangle$ of $Q^k|\gamma\rangle$. Let $Q|\gamma\rangle = \alpha|\gamma\rangle + \beta(U^{-1}|\tau\rangle)$, $Q(U^{-1}|\tau\rangle) = \lambda|\gamma\rangle + \delta(U^{-1}|\tau\rangle)$. Then

$Q^2|\gamma\rangle = (\alpha^2 + \beta\lambda)|\gamma\rangle + (\alpha + \delta)(U^{-1}|\tau\rangle)$......(1)

$Q^3|\gamma\rangle = (\alpha^3 + \beta\lambda(2\alpha + \delta))|\gamma\rangle + \beta(\alpha^2 + \alpha\delta + \delta^2 + \beta\lambda)(U^{-1}|\tau\rangle)$......(2)

$Q^4|\gamma\rangle = (\alpha^4 + \beta\lambda(3\alpha^2 + 2\alpha\delta + \delta^2) + (\beta\lambda)^2)|\gamma\rangle$

$\quad + \beta(\alpha^3 + \alpha^2\delta + \alpha\delta^2 + \delta^3 + 2(\alpha + \delta)\beta\lambda)(U^{-1}|\tau\rangle)$......(3)

Let $Q^k|\gamma\rangle = a_k|\gamma\rangle + b_k(U^{-1}|\tau\rangle)$, where $a_k$ and $b_k$ are the amplitudes in the initial state $|\gamma\rangle$ and the desired state $U^{-1}|\tau\rangle$, respectively. Then $Q^{k+1}|\gamma\rangle = Q(Q^k|\gamma\rangle) = a_kQ|\gamma\rangle + b_kQ(U^{-1}|\tau\rangle)$

$= (\alpha a_k + \lambda b_k)|\gamma\rangle + (\beta a_k + \delta b_k)(U^{-1}|\tau\rangle)$, clearly $a_{k+1} = (\alpha a_k + \lambda b_k)$ and $b_{k+1} = (\beta a_k + \delta b_k)$.

It is also the iterated formula for amplitude amplification for Grover’s and Long et al.’s and Hoyer’s algorithms and any other quantum search algorithm which preserves a two-dimensional vector space. Clearly it does not need to computer $Q^k(U^{-1}|\tau\rangle)$ to derive the iterated formula.

3.2 The precise formula for the amplitude

From the iterated formula above by induction $a_k$ and $b_k$ can be precisely written as the following polynomial in $(\beta\lambda)$, respectively. Let $[x]$ be the greatest integer which is or less than $x$.

$b_k = \beta(c_{k0} + c_{k1}(\beta\lambda) + c_{k2}(\beta\lambda)^2 + \ldots + c_{k([k-1]/2]}(\beta\lambda)^{([k-1]/2]}), \ldots(4)

where $c_{kj} = \sum_{n=k-1-2j}^{0} j^{(j)} k^{(k-1-2j-n)\alpha^n \delta^{k-2j-n}}$ and $t^{(j)}_{ki} = \binom{i+j} j \binom{k-i-j-1} j$.

$a_k = \alpha^k + d_{k1}(\beta\lambda) + d_{k2}(\beta\lambda)^2 + \ldots + d_{k[k/2]}(\beta\lambda)^{[k/2]} \ldots(5)

where $d_{kj} = \sum_{n=k-2j}^{0} j^{(j)} k^{(k-2j-n)\alpha^n \delta^{k-2j-n}}$, and $t^{(j)}_{ki} = \binom{i+j-1} j \binom{k-i-j} j$. Note that $\binom n0 = 1$, for any $n \geq 0$.

For Grover’s algorithm $(\beta\lambda) = \alpha - 1, \delta = 1$. Then $b_k$ can be written as $b_k = \beta r_k$, where $r_k$ is real.

Here it does not need to computer $Q^k(U^{-1}|\tau\rangle)$ to derive the precise formula above. Clearly it will save much more time to computer amplitude amplification in the desired state using the precise formula for $b_k$ than the kth power of the matrix which represents the operator $Q$. The formula is also the precise formula for the amplitude amplification for Grover’s and Long et al.’s and Hoyer’s algorithms and any other quantum search algorithm which preserves a two-dimensional vector space. From the precise formula for $b_k$, it is not hard to see the phase conditions in $\mathbb{H}$ are only sufficient.
For the detailed derivation of \( b_k \), please see appendix 3.

### 3.3 The non-symmetric effects of different rotating angles

Let us study the non-symmetric effects of different rotating angles of the initial state \( |\gamma\rangle \) and the desired state \( U^{-1}|\tau\rangle \) on the amplitude in the desired state. Clearly the norm of \( b_k \) contains the factor \(|\beta|\) which is \( 2|\cos \phi| \ |U_{\tau\gamma}| \). It is not hard to see that the effect of \( \phi \) on the amplitude in the desired state is greater than that of \( \theta \) when \( \theta \neq \phi \). It means that when \( \theta \neq \phi \) the effects of \( \theta \) and \( \phi \) on the amplitude in the desired state are not symmetric. For example, when \( \phi = \pi/2 \), then \( I_\tau = I, Q = -I, U = -I, U^{-1} U = -I, b_k = 0 \), it means that \( Q \) does nothing in the amplitude in the desired state except that it rotates the phase of the initial state \( |\gamma\rangle \) by angle \( \pi + 2\theta \). When \( \theta = \pi/2 \), then \( I_\gamma = I, Q = -I, U^{-1} U = -U^{-1} I, U, Q^k |\gamma\rangle = (-1)^k |\gamma\rangle + (\beta \sum_{i=0}^{k-1} (-1)^{k-1-i} \delta^i) U^{-1} |\tau\rangle \), \( |b_k| = 2|U_{\tau\gamma}| \ |\sin k(\pi/2 - \phi)\| \). The result in this subsection is also true for Long et al.’s algorithm.

### 3.4 The first-order approximate formula for the amplitude

Long et al. used many transformations and approximate operations to derive the approximate formula for the amplitude amplification[4]. Next let’s derive only by induction the first-order approximate formula for the amplitude \( b_k \) in the desired state \( U^{-1}|\tau\rangle \) using the iterated formula above though it is easy to derive it from the polynomial in \((\beta \lambda)\) of \( a_k \) and \( b_k \), please see (4) and (5) above. We only keep the first order of \( U_{\tau\gamma} \) in the amplitude in the state \( U^{-1}|\tau\rangle \). In \( b_{k+1} \), \( \beta \) contains the factor \( U_{\tau\gamma} \), so \( a_k \) should be approximated with the express without \( U_{\tau\gamma} \); \( \delta \) does not contain the term \( U_{\tau\gamma} \), so \( \delta b_k \) only contains the first order of \( U_{\tau\gamma} \) provided that \( b_k \) only contains the first order of \( U_{\tau\gamma} \). In \( a_{k+1} \), since \( \lambda \) contains the factor \( U^{\ast}_{\tau\gamma} \) and \( b_k \) contains the factor \( U_{\tau\gamma} \), \( \lambda b_k \) must contain \( |U_{\tau\gamma}|^2 \) and is omitted. Therefore \( a_{k+1} \) should be approximated by \( \sigma \ a_k \), that is, \( a_{k+1} = \sigma \ a_k \), to make \( a_{k+1} \) not contain factor \( U_{\tau\gamma} \). Let’s see how to approximate \( Q^k |\gamma\rangle \) by induction. Clearly

\[
Q|\gamma\rangle \doteq \sigma |\gamma\rangle + \beta(U^{-1}|\tau\rangle),
\]

\[
Q^2|\gamma\rangle \doteq \sigma^2 |\gamma\rangle + \beta(\sigma + \delta)(U^{-1}|\tau\rangle).
\]

Assume that \( Q^k |\gamma\rangle \doteq \sigma^k |\gamma\rangle + \beta(\sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i)(U^{-1}|\tau\rangle) \). Then \( Q^{k+1} |\gamma\rangle \doteq \sigma^{k+1} |\gamma\rangle + (\beta \sigma^k + \delta \beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i)(U^{-1}|\tau\rangle) = \sigma^{k+1} |\gamma\rangle + \beta(\sum_{i=0}^{k} \sigma^{k-i} \delta^i)(U^{-1}|\tau\rangle) \). Then by induction \( b_k \doteq \beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i \).
It is easy to verify that the approximate formula is just the first-order of $U_{r\gamma}$ in the precise formula for $b_k$. Please see the appendix 3. Clearly it does not need to computer $Q^k(U^{-1}|\tau\rangle)$ to derive the approximate formula above.

3.5 A mathematical proof of Grover’s algorithm being optimal among the algorithms with arbitrary phase rotations

Next let’s use the approximate formula to study its amplitude amplification and prove that Grover’s algorithm is optimal. Clearly $|\beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i| \leq 2k |U_{r\gamma}|$. We will prove that for any case the norm of amplitude in desired state $U^{-1}|\tau\rangle$ after $k$ operations of $Q$ is less than $2k |U_{r\gamma}|$ except Grover’s algorithm.

Case 1, $\sigma = \delta$, that is, $\theta = \phi$. In the case the amplitude $b_k \doteq 2k \cos \phi e^{i\phi} \sigma^{k-1} U_{r\gamma} \sigma$, $|b_k| \doteq 2k |\cos \phi| |U_{r\gamma}|$. When $\cos \phi \neq 0$, that is, $I_\gamma = I_\tau \neq I$, we obtain a quantum search algorithm that succeeds with certainty.

Case 1.1. When $\sigma = \delta = 1$, that is, $\theta = \phi = 0$, that is Grover’s algorithm, $b_k \doteq \beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i = 2k U_{r\gamma}$, (please see the appendix 1 to check it), the norm of the amplitude $|b_k| \doteq 2k |U_{r\gamma}|$. Let $2k |U_{r\gamma}| = 1$, we obtained the maximum probability for the desired state $U^{-1}|\tau\rangle$, in the case the optimal number of operations of $Q$ is $1/2 |U_{r\gamma}|$, when $|U_{r\gamma}|$ is taken as $1/\sqrt{N}$, the number is $\sqrt{N}/2$. Here the optimal number is less than Grover’s optimal number $\pi/4|U_{r\gamma}|$ evaluated in [4]. The optimal number of iteration steps obtained by Long et al. [3] is $\pi/4\beta$, where $|U_{r\gamma}| = \sin \beta$, so the optimal number also is almost $\pi/4|U_{r\gamma}|$. Please see the $|b_k|$ in the table 1.

| $\sqrt{N}/2$ | $U_{r\gamma} = 1/\sqrt{N}$ | $k$ | $|b_k|$ |
|----------------|-----------------------------|----|--------|
| 100 5 | 0.1 | 6 | 0.9375 |
| 400 10 | 0.05 | 12 | 0.9334 |
| 625 12 | 0.04 | 14 | 0.9010 |
| 900 15 | 1/30 | 17 | 0.9064 |

Case 1.2. When $\sigma = \delta \neq 1$, clearly $|\beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i| < 2k |U_{r\gamma}|$.

Case 2, $\sigma \neq \delta$, that is, $\theta \neq \phi$. Clearly $\sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i = \frac{\sigma^{k-1} - \delta^k}{\sigma - \delta}$. $|b_k| \doteq |\beta \sum_{i=0}^{k-1} \sigma^{k-1-i} \delta^i| = 2|\cos \phi| U_{r\gamma} \sqrt{\frac{1 - \cos 2k(\theta - \phi)}{1 - \cos 2(\theta - \phi)}} = 2|\cos \phi| U_{r\gamma} \| \frac{\sin k(\theta - \phi)}{\sin(\theta - \phi)} \|$. In the case $\sigma \neq \delta$, $\cos(\theta - \phi) \neq \pm 1$, by the induction on $k$, it is not hard to prove that $\left| \frac{\sin k(\theta - \phi)}{\sin(\theta - \phi)} \right| < k(k > 1)$, therefore $|b_k| \doteq$
From the cases 1 and 2, for Grover’s algorithm in the first-order approximate $|b_k| = 2k |U_{\tau\gamma}|$; for other cases $|b_k| < 2k |U_{\tau\gamma}|$. It proved that Grover’s algorithm is an optimal one with the form $-I_{\gamma}U^{-1}I_{\tau}U$. From above $|b_k| = \begin{cases} 2k |\cos \phi||U_{\tau\gamma}|, & \theta = \phi; \\ 2 |\cos \phi||U_{\tau\gamma}| \left| \frac{\sin k(\theta - \phi)}{\sin(\theta - \phi)} \right|, & \theta \neq \phi, \end{cases}$ clearly the approximate formula is simpler than Long et al.’s one [5].

3.6 The first-order approximate phase condition with different rotating angles

In [6] Long et al. studied the effects of imperfect phase inversion. In [9] Peter Hoyer thinks if $\theta \neq \phi$ and $|\phi - \phi| \leq c/\sqrt{N}$ for some approximate constant $c$ then the marked state can still be found by Long et al.’s algorithm with high probability. Here we will give the first-order approximate phase condition that $|\theta - \phi| < 2 |\cos \phi||U_{\tau\gamma}|$ and deduce when $\theta \neq \phi$ and $\theta$ and $\phi$ satisfy the condition then the desired state can still be found by the present algorithm.

Let $Max_k |b_k|$ be the maximal $|b_k|$ for any $k$. When $\theta \neq \phi$ and $|\theta - \phi|$ is small, $Max_k |b_k| \doteq 2 |\cos \phi||U_{\tau\gamma}|/|\theta - \phi|$. It means that $Max_k |b_k|$ is the inverse ratio of $|\theta - \phi|$ when $|\theta - \phi|$ is small. When $\cos \phi \neq 0$, let $|\theta - \phi| = 2l |\cos \phi||U_{\tau\gamma}|$. Then $Max_k |b_k| \doteq 1/l$. When $0 \leq l < 1$, that is, $|\theta - \phi| < 2 |\cos \phi||U_{\tau\gamma}|$, almost $Max_k |b_k| \doteq 1$; when $1 < l$, that is, $|\theta - \phi| > 2 |\cos \phi||U_{\tau\gamma}|$, $Max_k |b_k| \leq 1/l < 1$. Please see the following table 2. In the table 2 let $U_{\tau\gamma} = 1/\sqrt{N}$ and $\phi = 0$, where $N = 100, U_{\tau\gamma} = 0.1$. The experiments were done on IBM PC using MATLAB.

| $\theta$ | $k$ | $|b_k|$ |
|---------|-----|--------|
| 0.01    | 7   | 0.9899 |
| 0.02    | 8   | 0.9994 |
| 0.03    | 8   | 0.9930 |
| 0.04    | 100 | 0.9861 |
| 0.05    | 100 | 0.9525 |

When $\sigma \neq \delta$, clearly $\lim_{\theta \to \phi} 2 |\cos \phi||U_{\tau\gamma}| \left| \frac{\sin k(\theta - \phi)}{\sin(\theta - \phi)} \right| = 2k |\cos \phi||U_{\tau\gamma}|$. When $\phi = 0$, the limitation is $2k |U_{\tau\gamma}|$, which is just Grover’s algorithm.

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Appendix 1
For Grover’s algorithm, $Q = -I_1^\gamma U^{-1}I_2^\gamma U,$
\[ Q|\gamma\rangle = (1 - 4|U_{\tau\gamma}|^2)|\gamma\rangle + 2U_{\tau\gamma}U^{-1}|\tau\rangle \\
Q^2|\gamma\rangle = Q(Q|\gamma\rangle) = ((1 - 4|U_{\tau\gamma}|^2)^2 - 4|U_{\tau\gamma}|^2)|\gamma\rangle + (4U_{\tau\gamma} - 8U_{\tau\gamma}|U_{\tau\gamma}|^2)(U^{-1}|\tau\rangle) \\
Q^3|\gamma\rangle = Q(Q^2|\gamma\rangle) = ((1 - 4|U_{\tau\gamma}|^2)^3 - 12|U_{\tau\gamma}|^2 + 32|U_{\tau\gamma}|^4)|\gamma\rangle + (6U_{\tau\gamma} - 32U_{\tau\gamma}|U_{\tau\gamma}|^2 + 32U_{\tau\gamma}|U_{\tau\gamma}|^4)(U^{-1}|\tau\rangle)

**Appendix 2**

\[ Q = -I_1^\gamma V I_2^\gamma U. \] And note that $\langle\gamma|\gamma\rangle = 1,$ $\langle\tau|U|\gamma\rangle = U_{\tau\gamma}, \langle\gamma|U^{-1}|\tau\rangle = U_{\tau\gamma}$ (Since $U^{-1} = U^*$ and $\langle\gamma|U^*|\tau\rangle = \langle\tau|U|\gamma\rangle$). Then
\[ Q|\gamma\rangle = -I_1^\gamma V U|\gamma\rangle = -(I - 2|\gamma\rangle\langle\gamma|)V(I - 2|\tau\rangle\langle\tau|)U|\gamma\rangle \\
= -(V U)|\gamma\rangle + 2|\gamma\rangle\langle\gamma|V U|\gamma\rangle + 2U_{\tau\gamma}(V|\tau\rangle - 4U_{\tau\gamma}|\gamma\rangle\langle\tau|V|\gamma\rangle \\
= -(V U)|\gamma\rangle + 2(V U)|\gamma\rangle - 4U_{\tau\gamma}V_{\tau\gamma}|\gamma\rangle + 2U_{\tau\gamma}(V|\tau\rangle).
\]
\[ Q(U^{-1}|\tau\rangle) = -I_1^\gamma V I_2^\gamma U(U^{-1}|\tau\rangle) = -I_1^\gamma V I_2^\gamma |\tau\rangle = I_1 V |\tau\rangle \\
= (I - 2|\gamma\rangle\langle\gamma|)V|\tau\rangle = V|\tau\rangle - 2V_{\gamma\tau}|\gamma\rangle.
\]
\[ Q(V U)|\gamma\rangle = -I_1^\gamma V I_2^\gamma U(V V U)|\gamma\rangle = -(I - 2|\gamma\rangle\langle\gamma|)V(I - 2|\tau\rangle\langle\tau|)U(V U)|\gamma\rangle \\
= -(I - 2|\gamma\rangle\langle\gamma|)(V V U)|\gamma\rangle - 2V|\tau\rangle\langle\tau|U V U)|\gamma\rangle \\
= -(V V U)|\gamma\rangle + 2V|\tau\rangle\langle\tau|U V U)|\gamma\rangle + 2|\gamma\rangle\langle\gamma|V V U|\gamma\rangle - 4|\gamma\rangle\langle\gamma|V |\tau\rangle\langle\tau|UV U|\gamma\rangle \\
When VU is hermitian, then V V U = I, V U V = U^{-1} and V U V V = V^{-1}.

Then $Q(V U)|\gamma\rangle = -|\gamma\rangle + 2V_{\gamma\tau}^* (V|\tau\rangle) + 2|\gamma\rangle - 4V_{\gamma\tau} V_{\tau\gamma}^* |\gamma\rangle = (1 - 4|V_{\tau\gamma}|^2)|\gamma\rangle + 2V_{\gamma\tau}^* (V|\tau\rangle).
\]
\[ Q(V|\tau\rangle) = -I_1^\gamma V I_2^\gamma U(V|\tau\rangle) = -(I - 2|\gamma\rangle\langle\gamma|)V(I - 2|\tau\rangle\langle\tau|)U(V|\tau\rangle) \\
= -(I - 2|\gamma\rangle\langle\gamma|)(V V U)|\tau\rangle - 2V|\tau\rangle\langle\tau|U V U|\tau\rangle \\
= -(V V U)|\tau\rangle - 2V|\tau\rangle\langle\tau|U V U|\tau\rangle - 2|\gamma\rangle\langle\gamma|V V U|\tau\rangle + 4|\gamma\rangle\langle\gamma|V |\tau\rangle\langle\tau|UV U|\tau\rangle \\
Then $Q(V|\tau\rangle) = -U^{-1}|\tau\rangle + 2(U V)|\tau\rangle + (2U_{\gamma\tau}^* - 4V_{\gamma\tau} V_{\tau\gamma}^* |\gamma\rangle
\]

**Appendix 3**
The algorithm $Q = -I_1 U^{-1} U$, where $I_1 = I - 2 \cos \theta e^{i\theta} |\gamma\rangle\langle\gamma| |\tau\rangle$ and $I_2 = I - 2 \cos \phi e^{i\phi} |\tau\rangle\langle\tau| |\gamma\rangle.$
\[ Q|\gamma\rangle = -I_1 U^{-1} U|\gamma\rangle = -I_1 U^{-1} (I - 2 \cos \phi e^{i\phi} |\tau\rangle\langle\tau| |\gamma\rangle)U|\gamma\rangle \\
= -I_1 (U^{-1} U |\gamma\rangle - 2 \cos \phi e^{i\phi} U^{-1} |\tau\rangle\langle\tau| |\gamma\rangle)U|\gamma\rangle \\
= -I_1 (|\gamma\rangle - 2 \cos \phi e^{i\phi} U_{\tau\gamma}(U^{-1}|\tau\rangle)) \\
= -(I - 2 \cos \theta e^{i\theta} |\gamma\rangle\langle\gamma| |\gamma\rangle - 2 \cos \phi e^{i\phi} U_{\tau\gamma}(I - 2 \cos \theta e^{i\theta} |\gamma\rangle\langle\gamma|)(U^{-1}|\tau\rangle)) \\
= -(1 - 2 \cos \theta e^{i\theta} + 4 \cos \theta e^{i\theta} \cos \phi e^{i\phi} |U_{\tau\gamma}|^2 |\gamma\rangle + 2 \cos \phi e^{i\phi} U_{\tau\gamma}(U^{-1}|\tau\rangle). \\
Q(U^{-1}|\tau\rangle) = -I_1 U^{-1} I_2 U(U^{-1}|\tau\rangle) = -I_1 U^{-1} I_2 |\tau\rangle

respectively;...

Therefore, the diagonal elements 1, 2, 3, 4, ..., times 2 are 2, 4, 6, 8, ..., respectively; then they times 3 are 3, 6, 9, ..., respectively.

The following is the detailed derivation of the precise formula for the amplitude amplification. Let $Q^k|\gamma\rangle = a_k|\gamma\rangle + b_k(U^{-1}|\gamma\rangle)$, where $a_k$ and $b_k$ are the amplitudes in the state $|\gamma\rangle$ and the desired state $U^{-1}|\gamma\rangle$, respectively. Then

\[
\begin{align*}
b_5 &= \beta((\alpha^4 + \alpha^3\delta + \alpha^2\delta^2 + \alpha\delta^3 + \delta^4) + (3\alpha^2 + 4\alpha\delta + 3\delta^2)\beta\lambda + (\beta\lambda)^2) \\
a_5 &= \alpha^5 + (4\alpha^3 + 3\alpha^2\delta + 2\alpha\delta^2 + \delta^3)\beta\lambda + (3\alpha + 2\delta)(\beta\lambda)^2 \\
b_6 &= \beta((\alpha^5 + \alpha^4\delta + \alpha^3\delta^2 + \alpha^2\delta^3 + \alpha\delta^4 + \delta^5) + (4\alpha^3 + 6\alpha^2\delta + 6\alpha\delta^2 + 4\delta^3)\beta\lambda + 3(\alpha + \delta)(\beta\lambda)^2) \\
a_6 &= \alpha^6 + (5\alpha^4 + 4\alpha^3\delta + 3\alpha^2\delta^2 + 2\alpha\delta^3 + \delta^4)\beta\lambda + (6\alpha^2 + 6\alpha\delta + 3\delta^2)(\beta\lambda)^2 + (\beta\lambda)^3
\end{align*}
\]

From the iterated formula it is not hard to by induction show that $a_k$ and $b_k$ can be written as the following polynomial in $(\beta\lambda)$, respectively.

\[
b_k = \beta(c_{k0} + c_{k1}(\beta\lambda) + c_{k2}(\beta\lambda)^2 + ... + c_{k(k-1)/2}(\beta\lambda)^{(k-1)/2}), ...
\]

where \( c_{kj} = \sum_{n=k-1-2j-n}^{0} t_k^{(j)} n^k \delta^{k-1-2j-n} \).

\[
a_k = \alpha^k + d_{k1}(\beta\lambda) + d_{k2}(\beta\lambda)^2 + ... + d_{k(k/2)][(\beta\lambda)]^{(k/2)}}...
\]

where \( d_{kj} = \sum_{n=k-2j-n}^{0} t_k^{(j)} n^k \delta^{k-2j-n} \).

\( t_{ki} \) in the coefficients of \( \beta\lambda \) in $b_5, b_4, b_5, b_6, b_7$ constitute the following pyramid.

The table 3.

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 |   |   |   |   |   |
| 2 |   |   |   |   |   |
| 3 | 4 | 5 |   |   |   |
| 4 | 6 | 8 | 9 | 11 |   |
| 5 | 9 | 13 | 17 | 21 | 25 |

Note that the diagonal elements 1, 2, 3, 4, ..., can be represented by (\( \frac{1}{3} \)), (\( \frac{2}{3} \)), (\( \frac{3}{3} \)), (\( \frac{4}{3} \))...; the diagonal elements 1, 2, 3, 4, ... times 2 are 2, 4, 6, 8, ..., respectively; then they times 3 are 3, 6, 9, ..., respectively;...
For example, \( l_{70}^{(1)}, l_{71}^{(1)}, l_{72}^{(1)}, l_{73}^{(1)} \) and \( l_{74}^{(1)} \) in the coefficient \( c_{71} \) of \( \beta \lambda \) in \( b_7 \) can be represented by \((\frac{1}{3})(\frac{1}{3}), (\frac{1}{3})(\frac{1}{3}), (\frac{1}{3})(\frac{1}{3}) \) respectively.

\( l_{k}^{(1)} \), in the coefficients of \((\beta \lambda)^2 \) in \( b_5, b_6, b_7, b_8 \) constitute the following pyramid.

The table 4.

| 1 | 3 | 6 | 10 | 10 |
|---|---|---|----|----|
| 3 | 9 | 18 | 18 | 18 |
| 6 | 18 | 18 | 18 | 18 |
| 10 | 18 | 18 | 18 | 18 |
| 18 | 18 | 18 | 18 | 18 |
| 10 | 18 | 18 | 18 | 18 |
| 18 | 18 | 18 | 18 | 18 |
| 18 | 18 | 18 | 18 | 18 |
| 18 | 18 | 18 | 18 | 18 |

Note that the diagonal elements 1,3,6,10,..., can be represented by \((\frac{3}{3}), (\frac{3}{3}), (\frac{3}{3})\); the diagonal elements 1,3,6,... times 3 are 3,9,18,..., respectively; then they times 6 are 6,18,..., respectively.

For example, \( l_{70}^{(2)}, l_{71}^{(2)} \) and \( l_{72}^{(2)} \) in the coefficient \( c_{72} \) of \((\beta \lambda)^2 \) in \( b_7 \) can be also represented by \((\frac{3}{3})(\frac{1}{3}), (\frac{3}{3})(\frac{1}{3}) \) and \((\frac{1}{3})(\frac{1}{3})\) respectively.

\( l_{k}^{(1)} \), in the coefficients of \((\beta \lambda)^3 \) in \( b_7, b_8, b_9, b_{10} \) constitute the following pyramid.

The table 5.

| 1 | 4 | 10 | 20 |
|---|---|----|----|
| 4 | 4 | 40 | 40 |
| 10 | 40 | 40 | 20 |
| 20 | 40 | 40 | 20 |

Note that the diagonal elements 1,4,10,20,... can be represented by \((\frac{3}{3}), (\frac{3}{3}), (\frac{3}{3})\); the diagonal elements 1,4,10,... times 4 are 4,16,40,..., respectively; then they times 10 are 10, 40,..., respectively.

For example, \( l_{100}^{(3)}, l_{101}^{(3)}, l_{102}^{(3)} \) and \( l_{103}^{(3)} \) in the coefficient \( c_{103} \) of \((\beta \lambda)^3 \) in \( b_{10} \) can be also represented by \((\frac{3}{3})(\frac{6}{6}), (\frac{3}{3})(\frac{6}{6}), (\frac{6}{6})(\frac{3}{3})\) respectively.

Generally \( l_{ki}^{(j)} \) in the coefficients of \((\beta \lambda)^k \) in \( b_{2k+1}, b_{2k+2}, b_{2k+3}, b_{2k+4}, b_{2k+5} \) constitute the following pyramid.

The table 6.

| \((\frac{3}{3})^{(k)}\) | \((\frac{3}{3})^{(k+2)}\) | \((\frac{3}{3})^{(k+1)}\) | \((\frac{3}{3})^{(k+1)}\) | \((\frac{3}{3})^{(k+2)}\) | \((\frac{3}{3})^{(k+3)}\) | \((\frac{3}{3})^{(k+4)}\) |
|\((\frac{3}{3})^{(k)}\) | \((\frac{3}{3})^{(k+2)}\) | \((\frac{3}{3})^{(k+1)}\) | \((\frac{3}{3})^{(k+1)}\) | \((\frac{3}{3})^{(k+2)}\) | \((\frac{3}{3})^{(k+3)}\) | \((\frac{3}{3})^{(k+4)}\) |

Therefore we can conclude and prove by induction that \( l_{ki}^{(j)} = \binom{i+j}{k} \binom{k-j-1}{j} \). So we obtain the precise formula for the amplitude \( b_k \) in the desired state after operations of the algorithm \( Q \).

**Appendix 4**
The sufficient condition in which \((VU)\) and \((UV)\) are hermitian and all the diagonal terms of \((VU)\) and \((UV)\) are zero.

Let’s define the \(N \times N\) matrix \(P\). Let \(p_{ij}\) be any terms of \(P\), where \(p_{(2i-1)(2i)} = 1\), \(p_{(2i)(2i-1)} = 1\) and \(p_{ij} = 0\) otherwise. Clearly \(P\) is unitary and hermitian, \(p^2 = 1\), and all the diagonal terms of \(P\) are zero. It is not hard to see that \(P\) has the block form which is \(\text{diag}\{P_1, P_2, ..., P_m\}\), where \(m = N/2\) and \(P_i \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\) for \(i = 1, 2, ..., m\).

It is easy to verify that \((PV)\) means to interchange lines \((2k-1)\) and \((2k)\) of \(V\) and \((VP)\) means to interchange columns \((2k-1)\) and \((2k)\) of \(V\), where \(k = 1, 2, ..., N/2\).

Given that \(V\) is unitary. Then if \(U = V^+P\) then \(U\) is unitary and \((VU) = V(V^+P) = (VV^+)P = P\). AS well if \(V = U^+P\) then \((UV) = (UU^+)P = P\). From \(U = V^+P\), obtain \(U^+ = PV\). From \(V = U^+P\), obtain \(V = PVP\). Then we conclude the following sufficient condition.

Sufficient condition (Version 1). If \(V\) is unitary, \(V = PVP\) and \(U = V^+P\), then \((VU)\) and \((UV)\) are unitary and hermitian, and all the diagonal terms of \((VU)\) and \((UV)\) are zero.

Proof. From the discussion above \((VU) = P\). Since \(V = PVP\), \((UV) = (V^+P)(PVP) = V^+P^2VP = (V+V)P = P\). By the property of \(P\), clearly the lemma holds.

Let \(V\) has the block form \(\begin{pmatrix} V_{11} & V_{12} & \cdots & V_{14} \\ V_{21} & V_{22} & \cdots & V_{24} \\ \vdots & \vdots & \ddots & \vdots \\ V_{m1} & V_{m2} & \cdots & V_{mn} \end{pmatrix}\), where \(m = N/2\) and each \(V_{ij}\) is \(2 \times 2\) submatrix.

It is not hard to see that \(V = PVP\) if and only if \(V_{ij}\) is of the form \(\begin{pmatrix} a & b \\ b & a \end{pmatrix}\) for \(1 \leq i, j \leq m\).

From this we conclude the version 2 of the sufficient condition.

The sufficient condition (Version 2)

If \(V\) is unitary and each \(V_{ij}\) of the block form of \(V\) is of the form \(\begin{pmatrix} a & b \\ b & a \end{pmatrix}\), and \(U = V^+P\). Then \((VU)\) and \((UV)\) are unitary and hermitian, and all the diagonal terms of \((VU)\) and \((UV)\) are zero.

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