

Grover's Quantum Search Algorithm

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ABSTRACT. This paper is a written version of a one hour lecture given on Lov Grover's quantum database search algorithm. It is based on [5], [6], and [11].

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1. Problem definition

We consider the problem of searching an unstructured database of $N = 2^n$ records for exactly one record which has been specifically marked. This can be rephrased in mathematical terms as an oracle problem as follows:

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Label the records of the database with the integers

$$0, 1, 2, \dots, N - 1,$$

and denote the label of the unknown marked record by x_0 . We are given an **oracle** which computes the n bit binary function

$$f : \{0, 1\}^n \longrightarrow \{0, 1\}$$

defined by

$$f(x) = \begin{cases} 1 & \text{if } x = x_0 \quad (\text{"Yes"}) \\ 0 & \text{otherwise} \quad (\text{"No"}) \end{cases}$$

By calling the function f an **oracle** we mean that we have neither access to the internal workings of the function f , nor immediate access to all argument-function pairs $(x, f(x))$. The oracle f operates simply as a blackbox function, which we can query as many times as we like. But with each such query comes an associated computational cost.

Search Problem for an Unstructured Database. *Find the record labeled as x_0 with the minimum amount of computational work, i.e., with the minimum number of queries of the oracle f .*

From elementary probability theory, we know that if we examine k random¹ records, i.e., if we compute the oracle f for k randomly chosen records, then the probability of finding the record labeled as x_0 is k/N . Hence, *on a classical computer*, finding the unknown record label x_0 comes with the computational price tag of $O(N) = O(2^n)$ computational steps.

2. Two examples

The above search problem for an unstructured database is a fundamental and practical problem which appears in many different guises.

2.1. Example 1. Searching a city phone book.

For example, consider a city phone book containing N phone numbers [3]. Find the name associated with the phone number

$x_0 = (123) \quad 456 - 7890$

As mentioned earlier, the best classical algorithm for finding the associated name, say Jane Doe, would search through $N/2$ phone numbers (i.e., $O(N)$ phone numbers) on average before finding the name Jane Doe.

¹We are assuming the uniform probability distribution.

2.2. Example 2. A plaintext/ciphertext attack on DES.

As another example, consider a **plaintext/ciphertext attack** by brute force key search on a message encrypted with the **Data Encryption Standard (DES)**, where the key K is a 56 bit number.

Given the plaintext/ciphertext pair

PlainText	At0500BlowUpTheEmbassyAt
CipherText	xjejpwwziderkqlievmsfkfdlqye

crack the entire cipher by encrypting the PlainText

At0500BlowUpTheEmbassyAt

with each of the $N = 2^{56}$ keys

$$K = 0, 1, 2, \dots, 2^{56} - 1,$$

in turn, until the key K_0 is found that produces the CipherText

xjejpwwziderkqlievmsfkfdlqye

In other words, if

$$(P, C)$$

denotes the available plaintext/ciphertext pair, and if

$$K_0$$

denotes the key such that

$$DES(P, K_0) = C,$$

then the **oracle** is

$$f(K) = \begin{cases} 1 & \text{if } K = K_0 \text{ ("Yes")} \\ 0 & \text{otherwise ("No")} \end{cases}$$

3. The quantum mechanical perspective

As we have seen, any classical algorithm for searching an unstructured database of N records must take on average at least $O(N)$ computational steps. However, much to everyone's surprise, Lov Grover actually found a non-classical quantum algorithm for searching such a database even faster, with an average of $O(\sqrt{N})$ steps, and with an average total computational cost of $O(\sqrt{N} \lg N)$. Although this is not exponentially faster, it is indeed a significant speedup.

Let \mathcal{H}_2 be a 2 dimensional Hilbert space with orthonormal basis

$$\{|0\rangle, |1\rangle\};$$

and let

$$\{|0\rangle, |1\rangle, \dots, |N-1\rangle\}$$

denote the induced orthonormal basis of the Hilbert space

$$\mathcal{H} = \bigotimes_0^{n-1} \mathcal{H}_2 .$$

From the quantum mechanical perspective, the oracle function f is given as a blackbox unitary transformation U_f , i.e., by

$$\mathcal{H} \otimes \mathcal{H}_2 \xrightarrow{U_f} \mathcal{H} \otimes \mathcal{H}_2$$

$$|x\rangle \otimes |y\rangle \mapsto |x\rangle \otimes |f(x) \oplus y\rangle$$

where ‘ \oplus ’ denotes exclusive ‘OR’, i.e., addition modulo 2.²

Instead of U_f , we will use the computationally equivalent unitary transformation

$$I_{|x_0\rangle}(|x\rangle) = (-1)^{f(x)} |x\rangle = \begin{cases} -|x_0\rangle & \text{if } x = x_0 \\ |x\rangle & \text{otherwise} \end{cases}$$

That $I_{|x_0\rangle}$ is computationally equivalent to U_f follows from the easily verifiable fact that

$$U_f \left(|x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right) = (I_{|x_0\rangle}(|x\rangle)) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}},$$

and also from the fact that U_f can be constructed from a controlled- $I_{|x_0\rangle}$ and two one qubit Hadamard transforms. (For details, please refer to [12], [13].)

The unitary transformation $I_{|x_0\rangle}$ is actually an **inversion** [1] in \mathcal{H} about the hyperplane perpendicular to $|x_0\rangle$. This becomes evident when $I_{|x_0\rangle}$ is rewritten in the form

$$I_{|x_0\rangle} = I - 2|x_0\rangle\langle x_0|,$$

where ‘ I ’ denotes the identity transformation. More generally, for any unit length ket $|\psi\rangle$, the unitary transformation

$$I_{|\psi\rangle} = I - 2|\psi\rangle\langle\psi|$$

is an inversion in \mathcal{H} about the hyperplane orthogonal to $|\psi\rangle$.

²Please note that $U_f = (\nu \circ \iota)(f)$, as defined in sections 10.3 and 10.4 of [14].

4. Properties of the inversion $I_{|\psi\rangle}$

We digress for a moment to discuss the properties of the unitary transformation $I_{|\psi\rangle}$. To do so, we need the following definition.

DEFINITION 1. Let $|\psi\rangle$ and $|\chi\rangle$ be two kets in \mathcal{H} for which the bracket product $\langle\psi|\chi\rangle$ is a real number. We define

$$\mathcal{S}_{\mathbb{C}} = \text{Span}_{\mathbb{C}}(|\psi\rangle, |\chi\rangle) = \{\alpha|\psi\rangle + \beta|\chi\rangle \in \mathcal{H} \mid \alpha, \beta \in \mathbb{C}\}$$

as the sub-Hilbert space of \mathcal{H} spanned by $|\psi\rangle$ and $|\chi\rangle$. We associate with the Hilbert space $\mathcal{S}_{\mathbb{C}}$ a real inner product space lying in $\mathcal{S}_{\mathbb{C}}$ defined by

$$\mathcal{S}_{\mathbb{R}} = \text{Span}_{\mathbb{R}}(|\psi\rangle, |\chi\rangle) = \{a|\psi\rangle + b|\chi\rangle \in \mathcal{H} \mid a, b \in \mathbb{R}\},$$

where the inner product on $\mathcal{S}_{\mathbb{R}}$ is that induced by the bracket product on \mathcal{H} . If $|\psi\rangle$ and $|\chi\rangle$ are also linearly independent, then $\mathcal{S}_{\mathbb{R}}$ is a 2 dimensional real inner product space (i.e., the 2 dimensional Euclidean plane) lying inside of the complex 2 dimensional space $\mathcal{S}_{\mathbb{C}}$.

PROPOSITION 1. Let $|\psi\rangle$ and $|\chi\rangle$ be two linearly independent unit length kets in \mathcal{H} with real bracket product; and let $\mathcal{S}_{\mathbb{C}} = \text{Span}_{\mathbb{C}}(|\psi\rangle, |\chi\rangle)$ and $\mathcal{S}_{\mathbb{R}} = \text{Span}_{\mathbb{R}}(|\psi\rangle, |\chi\rangle)$. Then

- 1) Both $\mathcal{S}_{\mathbb{C}}$ and $\mathcal{S}_{\mathbb{R}}$ are invariant under the transformations $I_{|\psi\rangle}$, $I_{|\chi\rangle}$, and hence $I_{|\psi\rangle} \circ I_{|\chi\rangle}$, i.e.,

$I_{ \psi\rangle}(\mathcal{S}_{\mathbb{C}}) = \mathcal{S}_{\mathbb{C}}$	and	$I_{ \psi\rangle}(\mathcal{S}_{\mathbb{R}}) = \mathcal{S}_{\mathbb{R}}$
$I_{ \chi\rangle}(\mathcal{S}_{\mathbb{C}}) = \mathcal{S}_{\mathbb{C}}$	and	$I_{ \chi\rangle}(\mathcal{S}_{\mathbb{R}}) = \mathcal{S}_{\mathbb{R}}$
$I_{ \psi\rangle}I_{ \chi\rangle}(\mathcal{S}_{\mathbb{C}}) = \mathcal{S}_{\mathbb{C}}$	and	$I_{ \psi\rangle}I_{ \chi\rangle}(\mathcal{S}_{\mathbb{R}}) = \mathcal{S}_{\mathbb{R}}$

- 2) If $L_{|\psi^\perp\rangle}$ is the line in the plane $\mathcal{S}_{\mathbb{R}}$ which passes through the origin and which is perpendicular to $|\psi\rangle$, then $I_{|\psi\rangle}$ restricted to $\mathcal{S}_{\mathbb{R}}$ is a reflection in (i.e., a Möbius inversion [1] about) the line $L_{|\psi^\perp\rangle}$. A similar statement can be made in regard to $|\chi\rangle$.
- 3) If $|\psi^\perp\rangle$ is a unit length vector in $\mathcal{S}_{\mathbb{R}}$ perpendicular to $|\psi\rangle$, then

$$-I_{|\psi\rangle} = I_{|\psi^\perp\rangle}.$$

(Hence, $\langle\psi^\perp|\chi\rangle$ is real.)

Finally we note that, since $I_{|\psi\rangle} = I - 2|\psi\rangle\langle\psi|$, it follows that

PROPOSITION 2. If $|\psi\rangle$ is a unit length ket in \mathcal{H} , and if U is a unitary transformation on \mathcal{H} , then

$$UI_{|\psi\rangle}U^{-1} = I_{U|\psi\rangle}.$$

5. The method in Lov's “madness”

Let $H : \mathcal{H} \longrightarrow \mathcal{H}$ be the Hadamard transform, i.e.,

$$H = \bigotimes_0^{n-1} H^{(2)},$$

where

$$H^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

with respect to the basis $|0\rangle, |1\rangle$.

We begin by using the Hadamard transform H to construct a state $|\psi_0\rangle$ which is an equal superposition of all the standard basis states $|0\rangle, |1\rangle, \dots, |N-1\rangle$ (including the unknown state $|x_0\rangle$), i.e.,

$$|\psi_0\rangle = H|0\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle .$$

Both $|\psi_0\rangle$ and the unknown state $|x_0\rangle$ lie in the Euclidean plane $\mathcal{S}_{\mathbb{R}} = \text{Span}_{\mathbb{R}}(|\psi_0\rangle, |x_0\rangle)$. Our strategy is to rotate within the plane $\mathcal{S}_{\mathbb{R}}$ the state $|\psi_0\rangle$ about the origin until it is as close as possible to $|x_0\rangle$. Then a measurement with respect to the standard basis of the state resulting from rotating $|\psi_0\rangle$, will produce $|x_0\rangle$ with high probability.

To achieve this objective, we use the oracle $I_{|x_0\rangle}$ to construct the unitary transformation

$$Q = -HI_{|0\rangle}H^{-1}I_{|x_0\rangle},$$

which by proposition 2 above, can be rewritten as

$$Q = -I_{|\psi_0\rangle}I_{|x_0\rangle} .$$

Let $|x_0^\perp\rangle$ and $|\psi_0^\perp\rangle$ denote unit length vectors in $\mathcal{S}_{\mathbb{R}}$ perpendicular to $|x_0\rangle$ and $|\psi_0\rangle$, respectively. There are two possible choices for each of $|x_0^\perp\rangle$ and $|\psi_0^\perp\rangle$ respectively. To remove this minor, but nonetheless annoying, ambiguity, we select $|x_0^\perp\rangle$ and $|\psi_0^\perp\rangle$ so that the orientation of the plane $\mathcal{S}_{\mathbb{R}}$ induced by the ordered spanning vectors $|\psi_0\rangle, |x_0\rangle$ is the same orientation as that induced by each of the ordered bases $|x_0^\perp\rangle, |x_0\rangle$ and $|\psi_0\rangle, |\psi_0^\perp\rangle$. (Please refer to Figure 2.)

REMARK 1. *The removal of the above ambiguities is really not essential. However, it does simplify the exposition given below.*

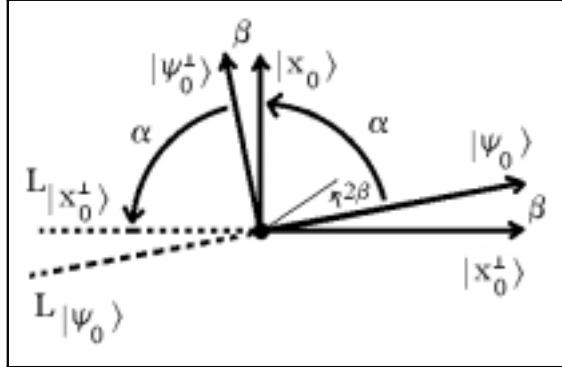


Figure 2. The linear transformation $Q|_{S_R}$ is a reflection in the line $L_{|x_0^\perp\rangle}$ followed by reflection in the line $L_{|\psi_0\rangle}$. By Theorem 1, this is the same as rotation by the angle 2β . Thus, $Q|_{S_R}$ rotates $|\psi_0\rangle$ by the angle 2β toward $|x_0\rangle$.

We proceed by noting that, by the above proposition 1, the plane S_R lying in \mathcal{H} is invariant under the linear transformation Q , and that, when Q is restricted to the plane S_R , it can be written as the composition of two inversions, i.e.,

$$Q|_{S_R} = I_{|\psi_0^\perp\rangle} I_{|x_0\rangle} .$$

In particular, $Q|_{S_R}$ is the composition of two inversions in S_R , the first in the line $L_{|x_0^\perp\rangle}$ in S_R passing through the origin having $|x_0\rangle$ as normal, the second in the line $L_{|\psi_0\rangle}$ through the origin having $|\psi_0^\perp\rangle$ as normal.³

We can now apply the following theorem from plane geometry:

THEOREM 1. *If L_1 and L_2 are lines in the Euclidean plane \mathbb{R}^2 intersecting at a point O , and if β is the angle in the plane from L_1 to L_2 , then the operation of reflection in L_1 followed by reflection in L_2 is just rotation by angle 2β about the point O .*

Let β denote the angle in S_R from $L_{|x_0^\perp\rangle}$ to $L_{|\psi_0\rangle}$, which by plane geometry is the same as the angle from $|x_0^\perp\rangle$ to $|\psi_0\rangle$, which in turn is the same as the angle from $|x_0\rangle$ to $|\psi_0^\perp\rangle$. Then by the above theorem $Q|_{S_R} = I_{|\psi_0^\perp\rangle} I_{|x_0\rangle}$ is a rotation about the origin by the angle 2β .

The key idea in Grover's algorithm is to move $|\psi_0\rangle$ toward the unknown state $|x_0\rangle$ by successively applying the rotation Q to $|\psi_0\rangle$ to rotate it around to $|x_0\rangle$.

³The line $L_{|x_0^\perp\rangle}$ is the intersection of the plane S_R with the hyperplane in \mathcal{H} orthogonal to $|x_0\rangle$. A similar statement can be made in regard to $L_{|\psi_0\rangle}$.

This process is called **amplitude amplification**. Once this process is completed, the measurement of the resulting state (with respect to the standard basis) will, with high probability, yield the unknown state $|x_0\rangle$. This is the essence of Grover's algorithm.

But how many times K should we apply the rotation Q to $|\psi_0\rangle$? If we applied Q too many or too few times, we would over- or undershoot our target state $|x_0\rangle$.

We determine the integer K as follows:

Since

$$|\psi_0\rangle = \sin \beta |x_0\rangle + \cos \beta |x_0^\perp\rangle ,$$

the state resulting after k applications of Q is

$$|\psi_k\rangle = Q^k |\psi_0\rangle = \sin [(2k+1)\beta] |x_0\rangle + \cos [(2k+1)\beta] |x_0^\perp\rangle .$$

Thus, we seek to find the smallest positive integer $K = k$ such that

$$\sin [(2k+1)\beta]$$

is as close as possible to 1. In other words, we seek to find the smallest positive integer $K = k$ such that

$$(2k+1)\beta$$

is as close as possible to $\pi/2$. It follows that

$$K = k = \text{round} \left(\frac{\pi}{4\beta} - \frac{1}{2} \right) = \left\lfloor \frac{\pi}{4\beta} \right\rfloor ,$$

where “*round*” is the function that rounds to the nearest integer, and where “[−]” denotes the floor function.

We can determine the angle β by noting that the angle α from $|\psi_0\rangle$ to $|x_0\rangle$ is complementary to β , i.e.,

$$\alpha + \beta = \pi/2 ,$$

and hence,

$$\frac{1}{\sqrt{N}} = \langle x_0 | \psi_0 \rangle = \cos \alpha = \cos \left(\frac{\pi}{2} - \beta \right) = \sin \beta .$$

Thus, the angle β is given by

$$\beta = \sin^{-1} \left(\frac{1}{\sqrt{N}} \right) \approx \frac{1}{\sqrt{N}} \quad (\text{for large } N) ,$$

and hence,

$$K = k = \left\lfloor \frac{\pi}{4 \sin^{-1} \left(\frac{1}{\sqrt{N}} \right)} \right\rfloor \approx \left\lfloor \frac{\pi \sqrt{N}}{4} \right\rfloor \quad (\text{for large } N).$$

6. Summary of Grover's algorithm

In summary, we provide the following outline of Grover's algorithm:

Grover's Algorithm	
STEP 0.	(Initialization) $ \psi\rangle \leftarrow H 0\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} j\rangle$ $k \leftarrow 0$
STEP 1.	Loop until $k = \left\lfloor \frac{\pi}{4 \sin^{-1}(1/\sqrt{N})} \right\rfloor \approx \left\lfloor \frac{\pi}{4} \sqrt{N} \right\rfloor$ $ \psi\rangle \leftarrow Q \psi\rangle = -H 0\rangle H _{x_0}\rangle \psi\rangle$ $k \leftarrow k + 1$
STEP 2.	Measure $ \psi\rangle$ with respect to the standard basis $ 0\rangle, 1\rangle, \dots, N-1\rangle$ to obtain the unknown state $ x_0\rangle$ with probability $\geq 1 - \frac{1}{N}$.

We complete our summary with the following theorem:

THEOREM 2. *With a probability of error*

$$Prob_E \leq \frac{1}{N},$$

Grover's algorithm finds the unknown state $|x_0\rangle$ at a computational cost of

$$O(\sqrt{N} \lg N)$$

PROOF.

Part 1. The probability of error $Prob_E$ of finding the hidden state $|x_0\rangle$ is given by

$$Prob_E = \cos^2[(2K+1)\beta],$$

where

$$\begin{cases} \beta = \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) \\ K = \left\lfloor \frac{\pi}{4\beta} \right\rfloor \end{cases},$$

and where “ $\lfloor - \rfloor$ ” denotes the floor function. Hence,

$$\frac{\pi}{4\beta} - 1 \leq K \leq \frac{\pi}{4\beta} \implies \frac{\pi}{2} - \beta \leq (2K+1)\beta \leq \frac{\pi}{2} + \beta$$

$$\implies \sin \beta = \cos\left(\frac{\pi}{2} - \beta\right) \geq \cos[(2K+1)\beta] \geq \cos\left(\frac{\pi}{2} + \beta\right) = -\sin \beta$$

Thus,

$$\text{Prob}_E = \cos^2[(2K+1)\beta] \leq \sin^2 \beta = \sin^2 \left(\sin^{-1} \left(\frac{1}{\sqrt{N}} \right) \right) = \frac{1}{N}$$

- Part 2. The computational cost of the Hadamard transform $H = \bigotimes_0^{n-1} H^{(2)}$ is $O(n) = O(\lg N)$ single qubit operations. The transformations $-I_{|0\rangle}$ and $I_{|x_0\rangle}$ each carry a computational cost of $O(1)$.

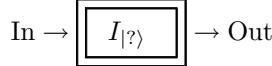
STEP 1 is the computationally dominant step. In **STEP 1** there are $O(\sqrt{N})$ iterations. In each iteration, the Hadamard transform is applied twice. The transformations $-I_{|0\rangle}$ and $I_{|x_0\rangle}$ are each applied once. Hence, each iteration comes with a computational cost of $O(\lg N)$, and so the total cost of **STEP 1** is $O(\sqrt{N} \lg N)$.

□

7. An example of Grover's algorithm

As an example, we search a database consisting of $N = 2^n = 8$ records for an unknown record with the unknown label $x_0 = 5$. The calculations for this example were made with OpenQuacks [15], an open source publically available quantum simulator Maple package developed at UMBC.

We are given a blackbox computing device



that implements as an oracle the unitary transformation

$$I_{|x_0\rangle} = I_{|5\rangle} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We cannot open up the blackbox → → to see what is inside. So we do not know what $I_{|x_0\rangle}$ and x_0 are. The only way that we can glean some information about x_0 is to apply some chosen state $|\psi\rangle$ as input, and then make use of the resulting output.

Using of the blackbox \rightarrow \rightarrow as a component device, we construct a computing device \rightarrow \rightarrow which implements the unitary operator

$$Q = -HI_{|0\rangle}HI_{|x_0\rangle} = \frac{1}{4} \begin{pmatrix} -3 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -3 \end{pmatrix}$$

We do not know what unitary transformation Q is implemented by the device \rightarrow \rightarrow because the blackbox \rightarrow \rightarrow is one of its essential components.

STEP 0. We begin by preparing the known state

$$|\psi_0\rangle = H|0\rangle = \frac{1}{\sqrt{8}}(1, 1, 1, 1, 1, 1, 1, 1)^{\text{transpose}}$$

STEP 1. We proceed to loop

$$K = \left\lfloor \frac{\pi}{4 \sin^{-1}(1/\sqrt{8})} \right\rfloor = 2$$

times in **STEP 1**.

ITERATION 1. On the first iteration, we obtain the unknown state

$$|\psi_1\rangle = Q|\psi_0\rangle = \frac{1}{4\sqrt{2}}(1, 1, 1, 1, 5, 1, 1, 1)^{\text{transpose}}$$

ITERATION 2. On the second iteration, we obtain the unknown state

$$|\psi_2\rangle = Q|\psi_1\rangle = \frac{1}{8\sqrt{2}}(-1, -1, -1, -1, 11, -1, -1, -1)^{\text{transpose}}$$

and branch to **STEP 2**.

STEP 2. We measure the unknown state $|\psi_2\rangle$ to obtain either

$$|5\rangle$$

with probability

$$\text{Prob}_{\text{Success}} = \sin^2((2K + 1)\beta) = \frac{121}{128} = 0.9453$$

or some other state with probability

$$Prob_{Failure} = \cos^2((2K+1)\beta) = \frac{7}{128} = 0.0547$$

and then exit.

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