Lesson 4. Quantum Algorithms: Grover Search and Applications

1. Introduction of Grover Search

You will see how this Lecture fits into the overall Course and know what you will learn the concepts of Grover search.

University of Tokyo

Special Lectures in Information Science II

Introduction of Near-Term Quantum Computing

情報科学科特別講義Ⅱ/量子計算論

4. Quantum Algorithms: Grover Search and Applications

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Discover Excellence. 東京大学 THE UNIVERSITY OF TOKYO

Course Schedule 2024

Date	Lecture Title	Lecturer	Date	Lecture Title	Lecturer
4/5	Invitation to the Utility era	Tamiya Onodera	6/7	Classical simulation (Clifford circuit, tensor network)	Yoshiaki Kawase
4/19	Quantum Gates, Circuits, and Measurements	Kifumi Numata	6/14	Quantum Hardware	Masao Tokunari
4/26	LOCC (Quantum teleportation/superdense coding)	Kifumi Numata	6/21	Quantum Circuit Optimization (transpiler)	Toshinari Itoko
5/10	Quantum Algorithms: Grover's algorithm	Atsushi Matsuo	6/28	Pauli twirling and Noise model (Pauli Transfer Matrix) Error mitigation (PEC, ZNE (PEA))	Toshinari Itoko
5/15 (Wed)	Quantum Algorithms: Phase estimation	Kento Ueda	7/5	Quantum Utility I (127Qubit GHZ)	Kifumi Numata
5/24	Quantum Algorithms: Variational Quantum Algorithms (VQA)	Takashi Imamichi	7/12	Quantum Utility II (Utility paper implementation)	Tamiya Onodera
5/30 (Thu)	Quantum simulation (Ising model, Heisenberg, XY model), Time evolution (Suzuki Trotter, QDrift)	Yukio Kawashima	7/19	Quantum Utility III (Krylov subspace expansion)	Yukio Kawashima

Lecture 4: Quantum Algorithms: Grover search and Applications

Agenda

- Introduction
- Grover search
- Quantum circuit for Grover search
- Qiskit Implementation

<u>Break</u>

- Geometric view of Grover Iteration
- Optimality of Grover search
- Summary
- Homework

Introduction

- The Grover search* is a quantum search algorithm.
  - Searching an unsorted database is often used as an example.
  - Also, it can be used to speed up many classical algorithms that use search algorithms
- Searching problem: Find ω from a list *L*
  - *L* is a list of size *N*, and ω is called the answer (or the "good" index).
- *How can we find ω from the list L?*
  - In classical computation, check each element of *L* until we find the answer.
    - In the worst case, Need $O(N)$ times.
  - In quantum computation, use Grover search!
    - Need $O(\sqrt{N})$ times.
- Quadratic speed up, <u>not exponential.</u>

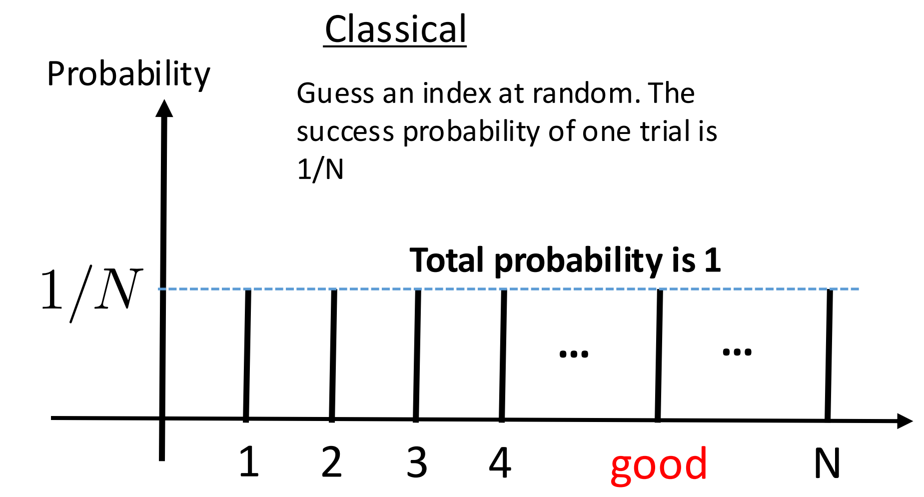
* Grover, Lov K. "A fast quantum mechanical algorithm for database search." *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*. 1996.

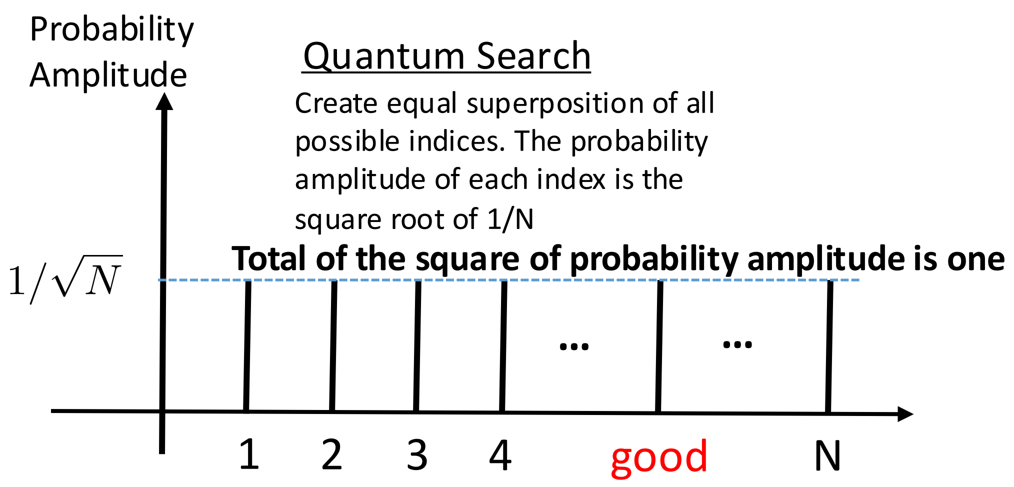
2. Classical and Quantum Search Algorithm

Grover Search is one of the quantum search algorithms. In quantum algorithms, a superposition state of all indices is created, and by using an oracle, it is possible to efficiently amplify the "good" state by utilizing probability amplitudes. You can learn the differences between Classical Search Algorithms and Quantum Search Algorithms and gain an understanding of Quantum Search Algorithms.

Classical and Quantum Search Algorithm

- **Searching Problem**
  - Find a good index *i* from N possible indices
  - Suppose we are given a black box that can answer whether index *i* is "good" or not. The black box is often called an "oracle".
- **Classical Search Algorithm**
  - Pick an index from 1～N at random. Ask the oracle with the index
  - The success probability is 1/N (if there is exactly one good index)
- **Quantum Search Algorithm**
  - Ask a quantum oracle with the superposition of all indices
  - With a query to the quantum oracle, the success probability is still 1/N, but before the measurement, the probability amplitude is 1/√N





Probability and Probability Amplitudes

- Success probabilities of classical algorithms
  - If one trial has success probability 1/N, k trials have success probability ~ k/N
  - Need to repeat k times up to the same order N
- Probability amplitude of quantum algorithms
  - Create a quantum superposition of all possible indices

$$\frac{1}{\sqrt{N}}|0\rangle + \frac{1}{\sqrt{N}}|1\rangle + \ldots + \frac{1}{\sqrt{N}}|N-1\rangle$$

  - Query the oracle to mark the bad/good indices and store the result in the second register

$$\frac{1}{\sqrt{N}}|0\rangle|\mathrm{bad}\rangle + \frac{1}{\sqrt{N}}|1\rangle|\mathrm{bad}\rangle + \ldots + \frac{1}{\sqrt{N}}|i\rangle|\mathrm{good}\rangle + \ldots + \frac{1}{\sqrt{N}}|N-1\rangle|\mathrm{bad}\rangle$$

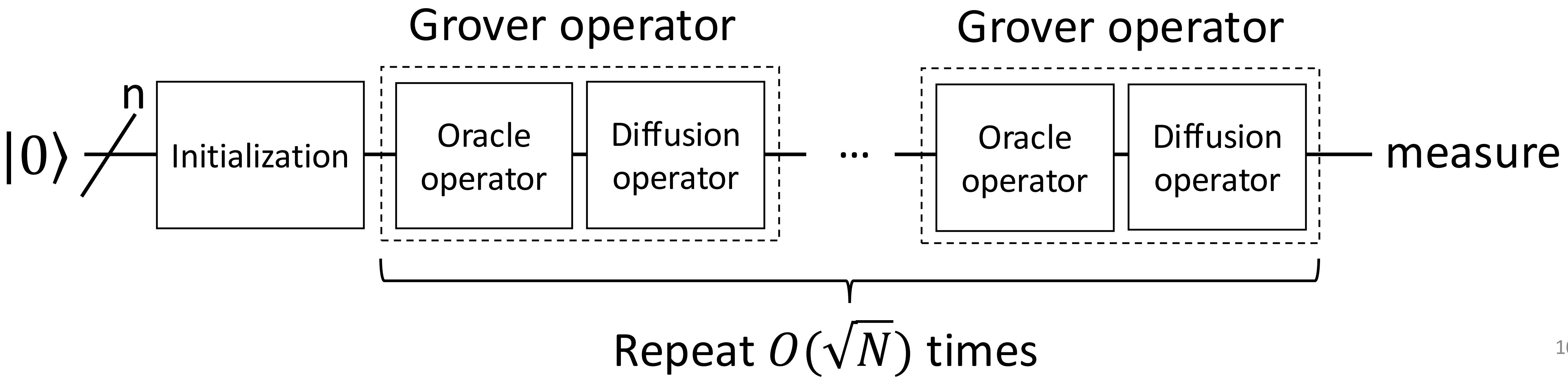
  - If we measure right after that, the result is similar to the classical algorithm
  - But, if we can add/gather the probability amplitudes, we may be able to amplify the good states quadratically faster
    - k repetitions of probability amplitudes resulting in $\frac{k}{\sqrt{N}}$ with success probability $\frac{k^2}{N}$
    - Only need to repeat up to the same order of the square root of N

3. What is Grover Search?

Grover Search consists of three parts: 1. Initialization, 2. Application of the Oracle Operator, and 3. Application of the Diffusion Operator, with steps 2 and 3 being repeated. You can learn the details of each step in Grover Search.

Overview

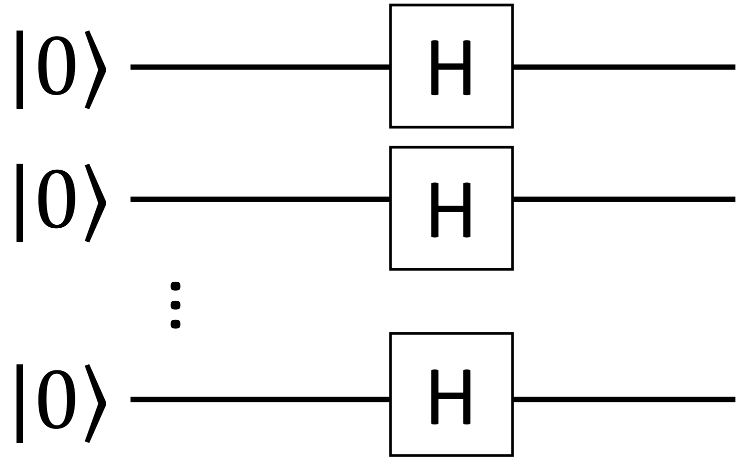
- The Grover search consists of three parts.
    1. Initialization
    2. Apply an Oracle operator
    3. Apply a Diffusion operator
- Repeat above 2 and 3 $O(\sqrt{N})$ times after initialization.



Initialization

- Create the superposition of all possible states $|00 \ldots 0\rangle \ldots |11 \ldots .1\rangle$ with equal amplitudes

- Apply Hadamard (H) gates to each qubit.



- The state will change to $|s\rangle = \sum_{x\in\{0,1\}^n}^{n} \frac{1}{\sqrt{2^n}} |x\rangle$ from $|00 \ldots 0\rangle$

Oracle operator

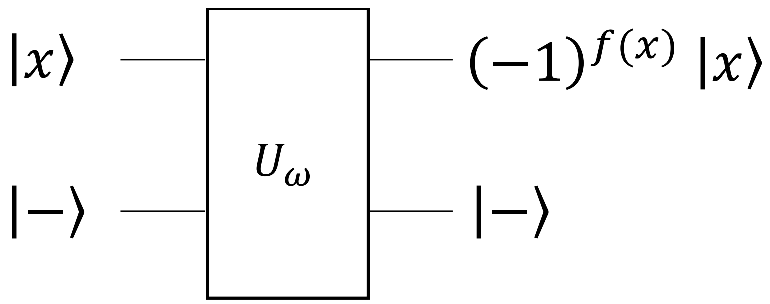
- Use the oracle in the oracle operator.
- Oracle: It's a black box function $f(x)$ as follows

$$\begin{cases} f(x) = 1 \ \text{ for } x = \omega, \\ f(x) = 0 \ \text{ for } x \neq \omega. \end{cases}$$

- Oracle operator: It's a black box operator U_ω as follows

$$U_\omega|x\rangle = (-1)^{f(x)}|x\rangle \qquad \begin{cases} U_\omega|x\rangle = -|x\rangle \ \text{ for } x = \omega, \\ U_\omega|x\rangle = \quad |x\rangle \ \text{ for } x \neq \omega. \end{cases}$$

- It changes the phase of $|x\rangle$ if $x = \omega$ by using a phase kickback.
  - I will explain in more detail later.



But… How can we make it? When we do not know the answer?

- I will explain in more detail later.

Diffusion operator

the superposition of all possible states with equal amplitudes. $(2^n = N)$

$$|s\rangle = N^{-1/2} \sum_{i\in\{0,1\}^n}^{n} |i\rangle$$

$$\langle s| = N^{-1/2} \sum_{j\in\{0,1\}^n}^{n} \langle j|$$

$$\langle j|i\rangle = \delta_{ij}$$

$$\langle \alpha \rangle = N^{-1} \sum_k \alpha_k$$

- Diffusion operator: $U_s = 2|s\rangle\langle s| - I$
- An Operator for the Inversion about the mean.
  - What does it mean?

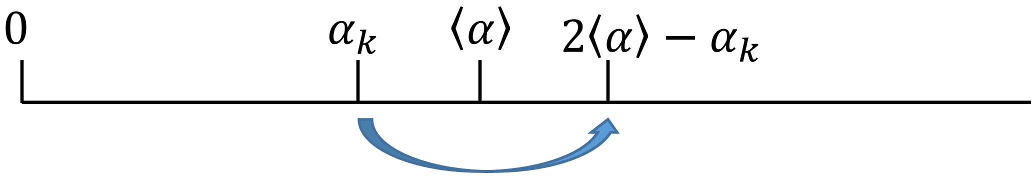
$$(2|s\rangle\langle s| - I\,) \sum_k \alpha_k\,|k\rangle$$

$$= 2N^{-1} \sum_{i,j,k} \alpha_k\,|i\rangle\langle j|k\rangle - \sum_k \alpha_k\,|k\rangle$$

$$= 2N^{-1} \sum_{i,k} \alpha_k\,|i\rangle - \sum_k \alpha_k\,|k\rangle$$

Arrange i and k since $2\langle\alpha\rangle$ is just a scalar

$$= \sum_k (2\langle\alpha\rangle - \alpha_k)\,|k\rangle$$



4. Example of 2-qubit and n-qubit Grover search

You can learn how Grover Search is executed with 2 qubits and n qubits, and how many iterations are required.

Example of 2-qubit Grover search

- Suppose ω is 2
- Initializing: Obtain the super position of all the possible states with equal amplitudes

$$|s\rangle = \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|\omega\rangle + \frac{1}{2}|11\rangle$$

- Apply an Oracle operator: Changes the phase of ω

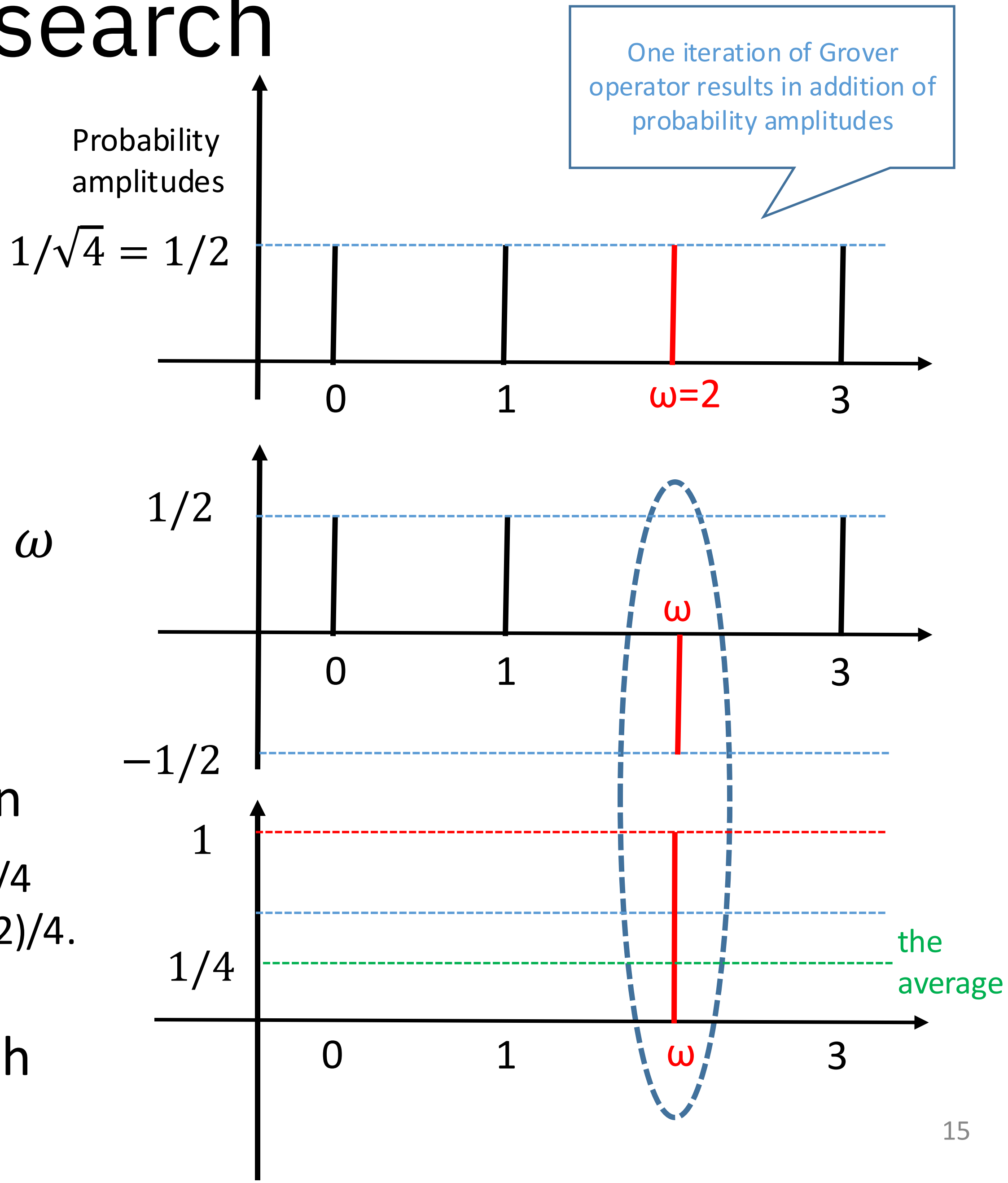
$$U_\omega|s\rangle = \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle - \frac{1}{2}|\omega\rangle + \frac{1}{2}|11\rangle$$

- Apply a Diffusion operator: Inversion about mean

$$U_s U_\omega|s\rangle = 0|00\rangle + 0|01\rangle + 1|\omega\rangle + 0|11\rangle$$

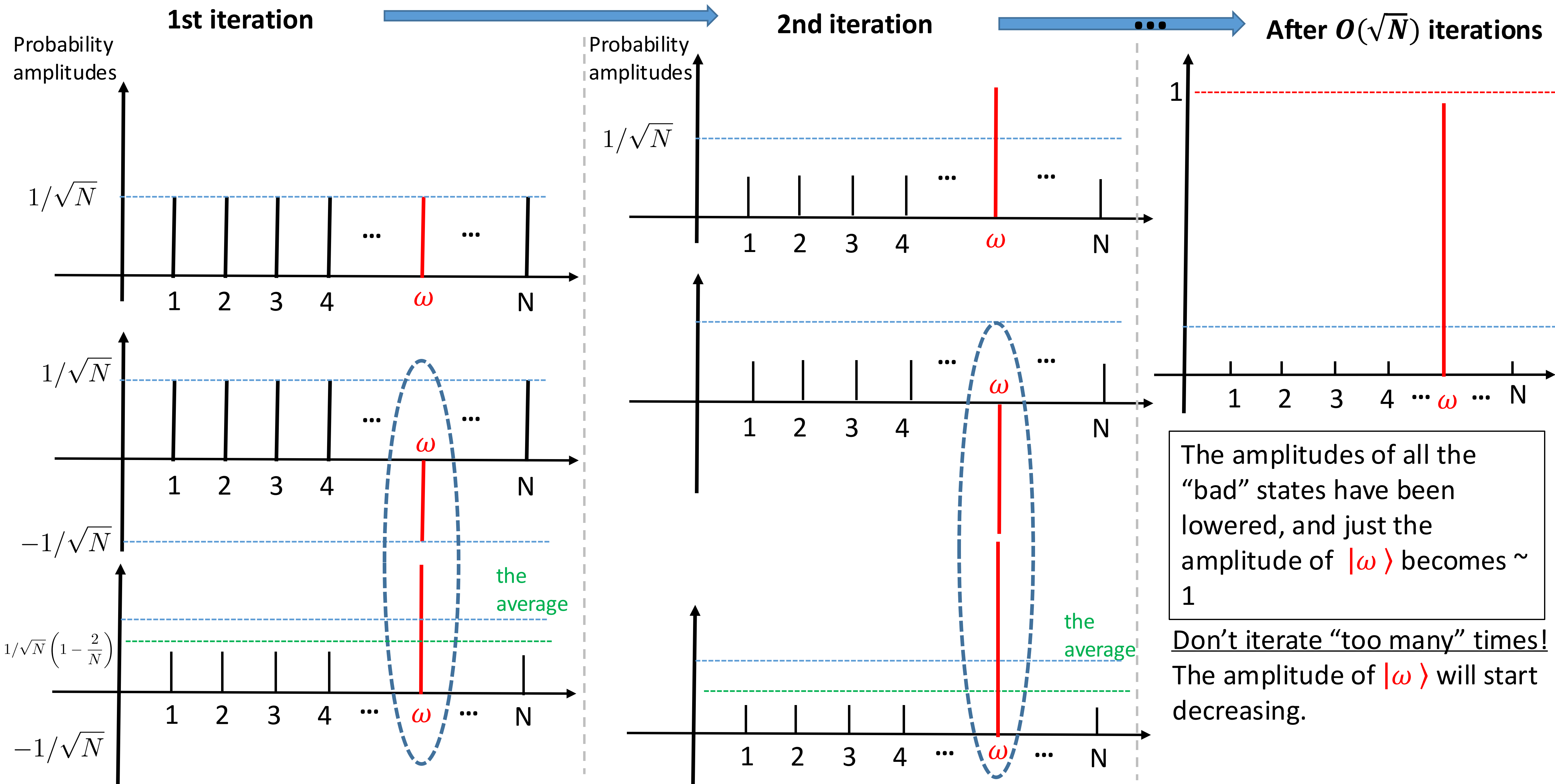
The average is 1/4 since (3*1/2 -1/2)/4.

<u>Only 1 iteration</u> is needed for 2-qubit Grover search



n-qubit Grover search

Good stateのインデックスをiからオメガに変更



The amplitudes of all the "bad" states have been lowered, and just the amplitude of $|\omega\rangle$ becomes ~ 1

<u>Don't iterate "too many" times!</u>

The amplitude of $|\omega\rangle$ will start decreasing.

5. Quantum circuit for Grover search

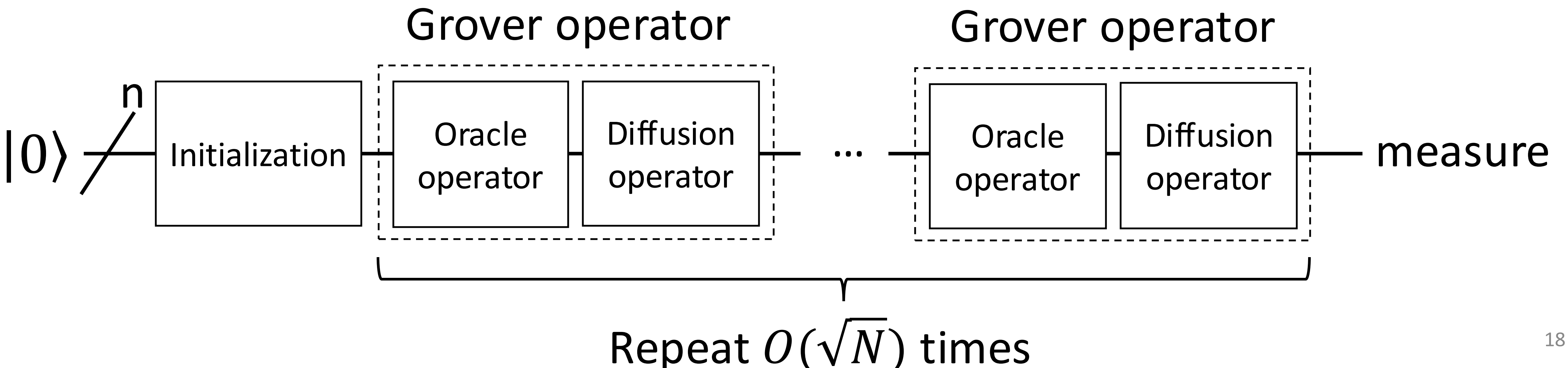
To implement Grover Search, it is necessary to construct the Oracle Operator and the Diffusion Operator, which correspond to each step. You can learn about the overview of each step and its correspondence to quantum circuits.

How to create Quantum circuit for Grover search?

- Initialization: Apply Hadamard (H) gates to each qubit (easy)
- Diffusion operator: create $U_s = 2|s\rangle\langle s| - I$ (sounds possible)
- Oracle operator: create $U_\omega|x\rangle = (-1)^{f(x)}|x\rangle$
  How can we make it? When we don't know the answer? (impossible?)
  If we can create the oracle, that means we know the answer, right?

Wrong!

There is a clear distinction between knowing the answer and being able to recognize the answer



6. How to create an oracle?

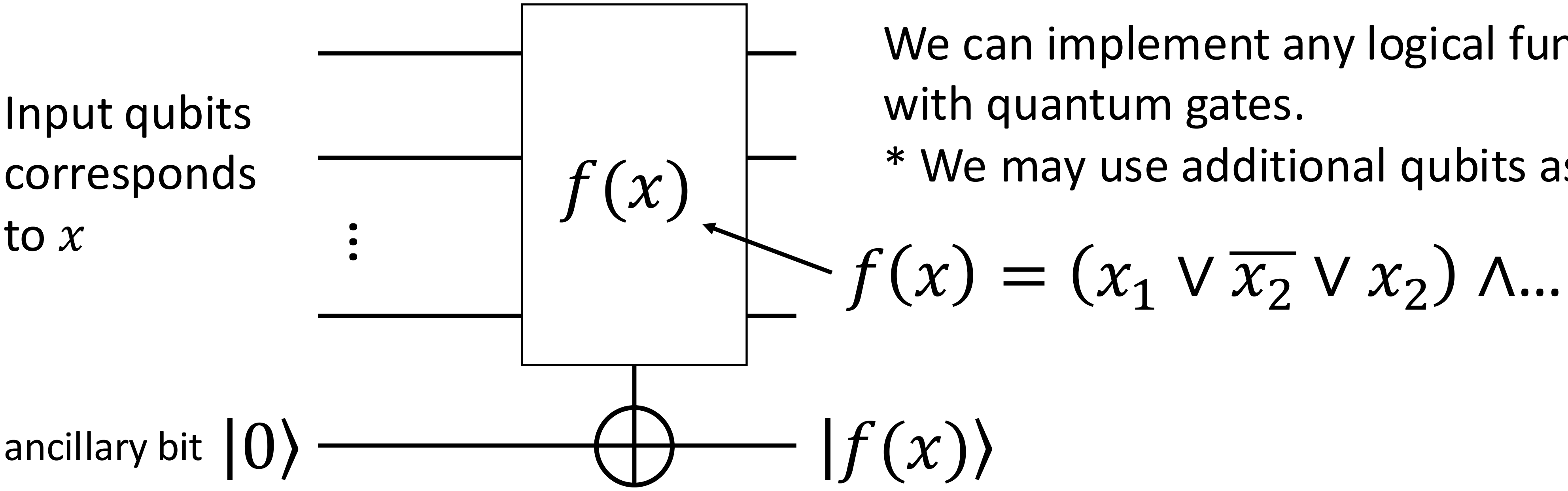
To implement Grover Search, it is necessary to construct the Oracle Operator and the Diffusion Operator, which correspond to each step. You can learn how to create the oracle when designing a quantum circuit for Grover Search.

How to create an oracle?

- An oracle is black box function $f(x)$ as follows

$$\begin{cases} f(x) = 1 \ \text{for} \ x = \omega, \\ f(x) = 0 \ \text{for} \ x \neq \omega. \end{cases}$$

- How to create it?
  - → Just implement $f(x)$ to the quantum circuit!



We can implement any logical function $f(x)$ with quantum gates.

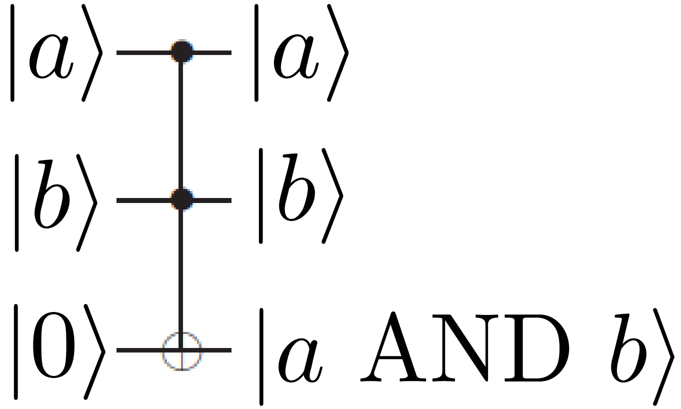
* We may use additional qubits as registers.

Reversible Boolean gates

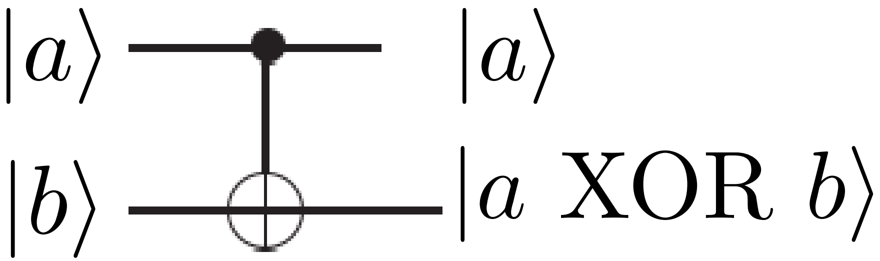
For *a, b* in *{0, 1}* (i.e., binaries), we can see compute the following operations with reversible gates.

NOT gate

AND gate



XOR gate



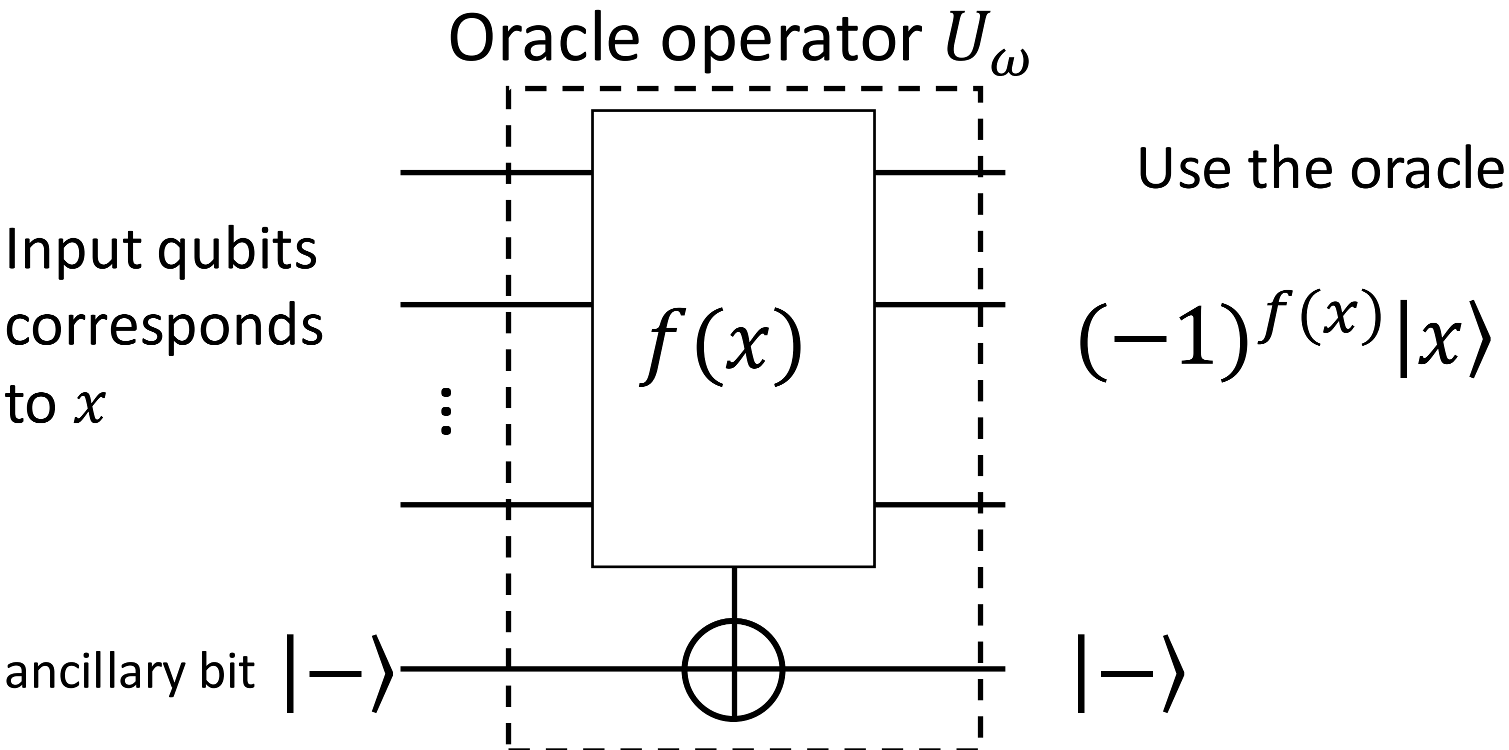
CCNOT gate (Toffoli gate) is a conditional gate that performs an X-gate on target bit (q2), if the two control qubits (q1, q0) are |11>.

How to create Oracle operator

- Oracle operator: a black box operator U_ω as follows.
  It changes the <u>phase</u> of $|x\rangle$ if $x = \omega$ by using a phase kick back.

$$U_\omega|x\rangle = (-1)^{f(x)}|x\rangle$$

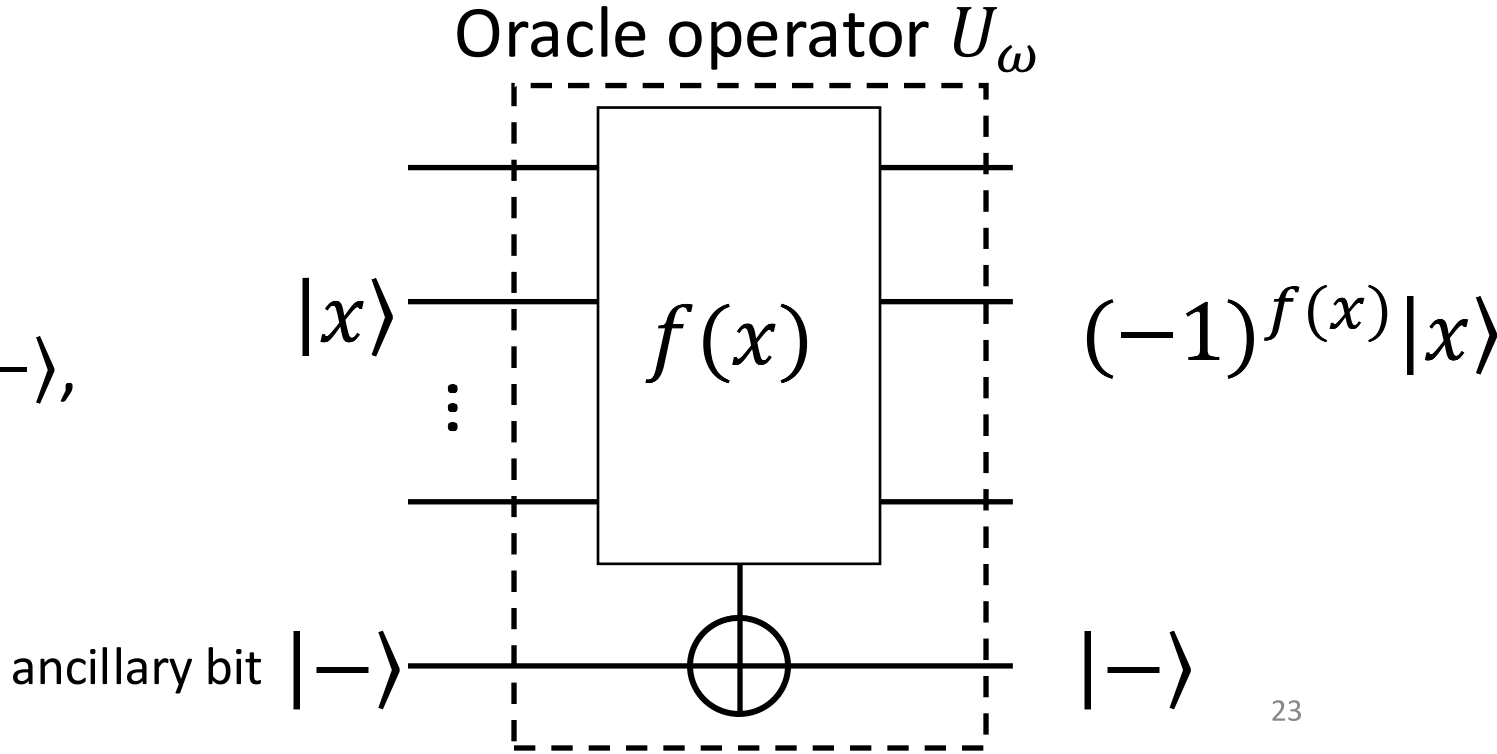
$$\begin{cases} U_\omega|x\rangle = -|x\rangle \ \text{ for } x = \omega, \\ U_\omega|x\rangle = \quad |x\rangle \ \text{ for } x \neq \omega. \end{cases}$$



Use the oracle and a phase kickback!

Phase kickback

- $|-\rangle$ is an eigenvector of the matrix representing an X gate, with an eigenvalue of -1.
  - $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$
  - A matrix of an X gate is $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
  - $X|-\rangle = -1 * |-\rangle$
- When we apply an X gate to $|-\rangle$, the state remains unchanged but we obtain a phase of -1.



7. How to create diffusion operator?

To implement Grover Search, it is necessary to construct the Oracle Operator and the Diffusion Operator, which correspond to each step. You can learn how to create the diffusion operator when designing a quantum circuit for Grover Search.

How to create diffusion operator?

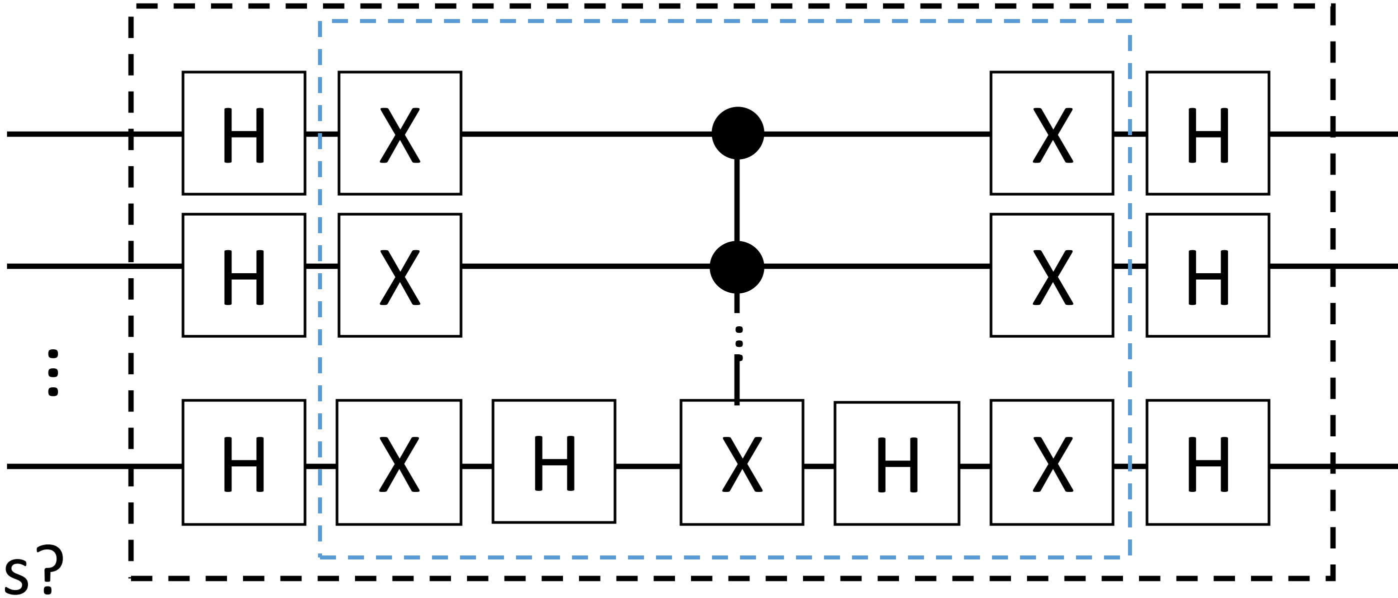
$|s\rangle = N^{-1/2} \sum_{i\in\{0,1\}^n}^{n} |i\rangle$

- Diffusion operator: $U_s = 2|s\rangle\langle s| - I$
- $2|s\rangle\langle s| - I = H^{\otimes n}(2|0\rangle\langle 0| - I)H^{\otimes n}$
- We consider the following operator
    - Equal to $(2|0\rangle\langle 0| - I)$ *up to global phase*

HH=I
Since an H gate is self-inverse

$$-(2|0\rangle\langle 0| - I) = \begin{bmatrix} -1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$$

Diffusion operator U_s

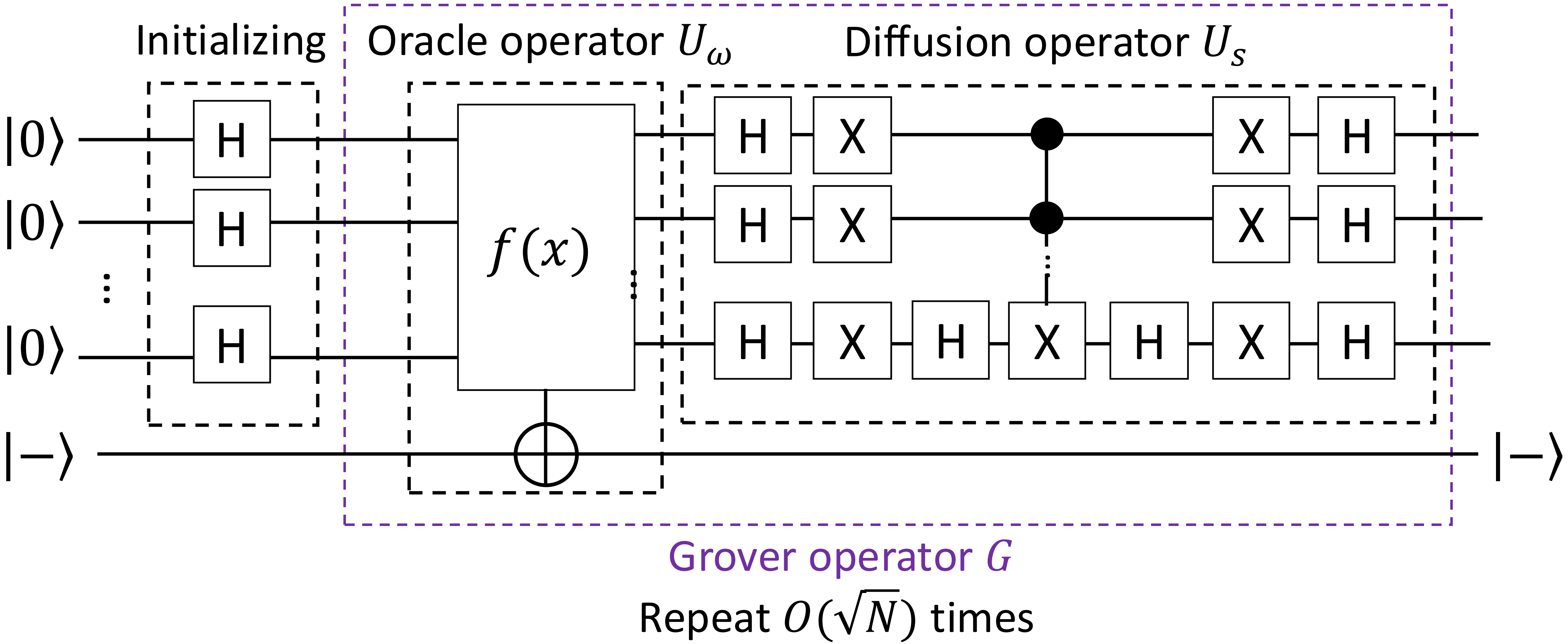


$-(2|0\rangle\langle 0| - I)$

- Looks similar to Controlled-Z gates?
    - Changes a phase of $|00 \dots 0\rangle$

Quantum circuit for Grover search

- By combining those circuit, we obtain a quantum circuit as follows.

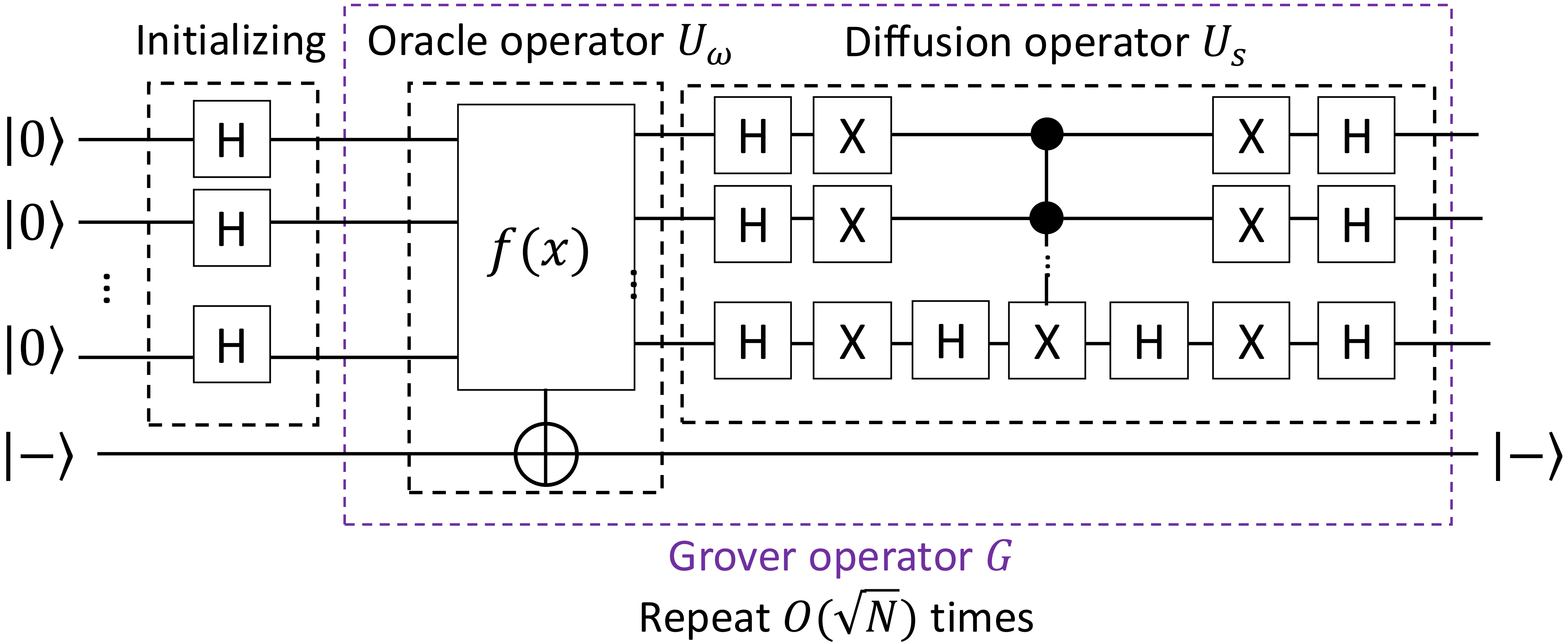


8. Creation of Quantum circuit for Grover search

You can learn how the Quantum Circuit for Grover Search is ultimately completed by combining the Oracle and the Diffusion Operator.

Quantum circuit for Grover search

- By combining those circuit, we obtain a quantum circuit as follows.



13. Geometric view of Grover Iteration

In Grover Search, repeating the iterations too many times is not appropriate. You will learn why excessive iterations should be avoided and how to determine the optimal number of iterations. Additionally, this lecture touches on the summary of these concepts.

“Good” vector and “bad” vector

- A quantum state is represented as a vector. We can always represent it as a weighted sum of other orthogonal vectors.

$$|\psi\rangle = \alpha\,|B\rangle + \beta\,|G\rangle = \gamma\,|\phi\rangle + \delta\,|\phi^{\perp}\rangle$$

- We can explain the behavior of Grover iterations as rotations. The vector is moved towards the space of the “good” vector.
  - “good” vector: $|\omega\rangle$ (“good” state)
  - ”bad” vector: spans perpendicular to $|\omega\rangle$, which is obtained from $|s\rangle$ by removing $|\omega\rangle$ and rescaling them.

$$|\psi\rangle = \cos\theta|bad\rangle + \sin\theta\,|good\rangle,$$

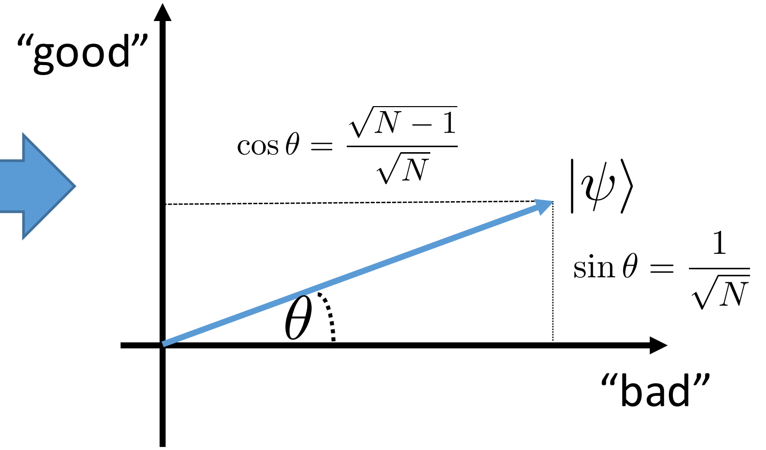
$$\cos^2\theta + \sin^2\theta = 1$$

Grover iteration explained with rotations of vectors

- **The initial state**

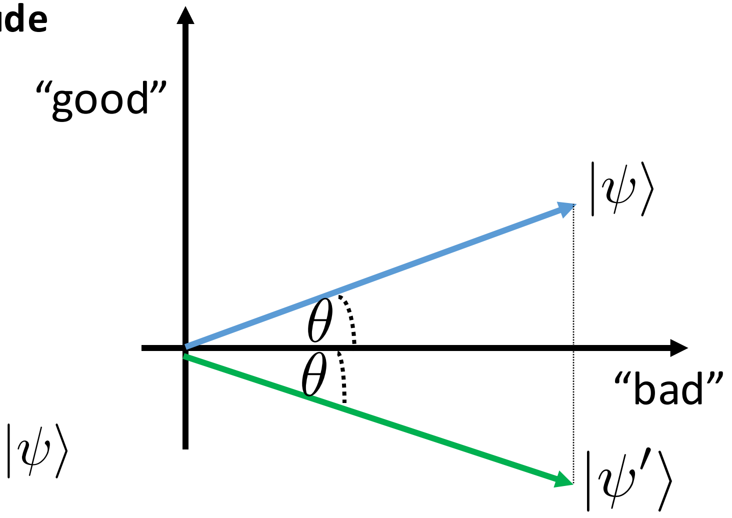
Note that $\sin\theta = \frac{1}{\sqrt{N}}$, $\cos\theta = \frac{\sqrt{N-1}}{\sqrt{N}}$

$$|\psi\rangle = \frac{1}{\sqrt{N}}|0\rangle + \frac{1}{\sqrt{N}}|1\rangle + \ldots + \frac{1}{\sqrt{N}}|N\rangle = \cos\theta\,|\text{bad}\rangle + \sin\theta\,|\text{good}\rangle$$

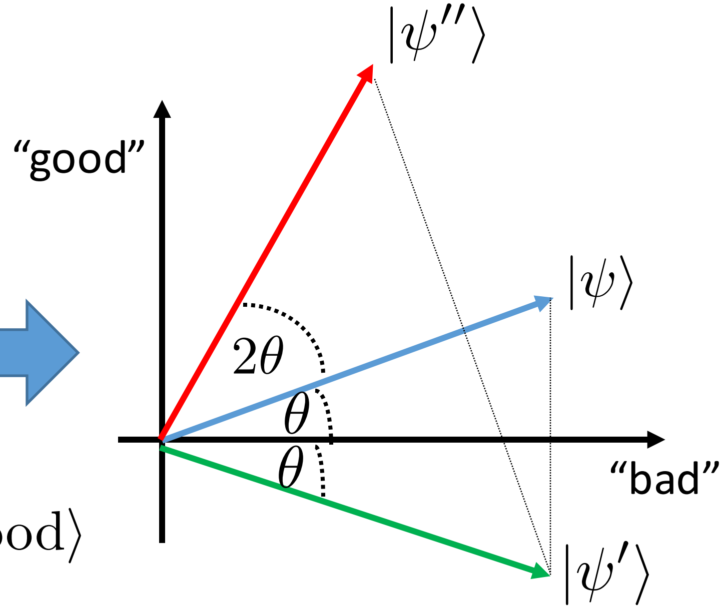


- **The oracle operator flips the probability amplitude of the good vector and leaves the bad one.**

$$U_\omega|\psi\rangle = |\psi'\rangle = \cos\theta\,|\text{bad}\rangle - \sin\theta\,|\text{good}\rangle$$



- **The diffusion operator flips the probability amplitude over the initial vector** $|\psi\rangle$



- **We have rotated the initial state by the angle 「2θ」 towards the "good" vector space.**

$$|\psi''\rangle = \cos(3\theta)\,|\text{bad}\rangle + \sin(3\theta)\,|\text{good}\rangle$$

The number of the optimal iteration

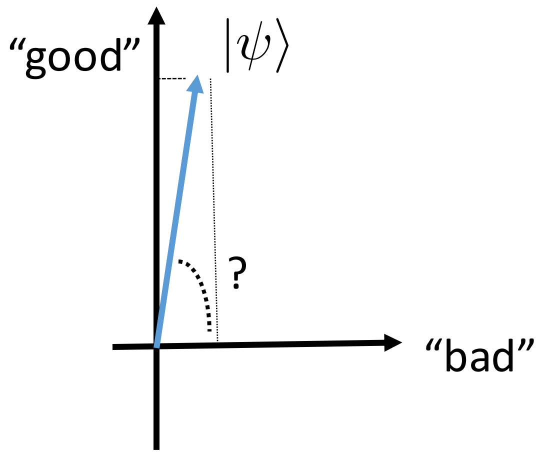
- After k iterations, the state will be $(U_s U_\omega)^k |s\rangle = \cos(2k+1)\theta\,|bad\rangle + \sin(2k+1)\theta\,|good\rangle$
- When k is $\mathrm{R} = \mathrm{ClosestInteger}\left(\frac{\pi}{4\theta} - \frac{1}{2}\right)$, $(U_s U_\omega)^k |s\rangle$ will be the closest to $|good\rangle$
    - ClosestInteger(x) means the closest integer to x
    - when (2k + 1)θ is π/2, the amplitude of ”good” will be 1
- Estimate the upper bound of R

using $\theta \geq \sin\theta = \frac{1}{\sqrt{N}}$

$$R \leq \left(\frac{\pi}{4\theta} - \frac{1}{2}\right) + 1 = \frac{\pi}{4\theta} + \frac{1}{2} \leq \frac{\pi}{4}\sqrt{N} + \frac{1}{2}$$

R is at most $O(\sqrt{N})$.

How many times do you need to repeat?



Summary of Geometric view of Grover iteration

- The success probability before applying the Grover operator is

$$\| \sin(\theta) \|^2 = \frac{1}{N}$$

- One step of Grover iterations rotates the vector by the angle 2θ towards the good space, and k steps of the iterations result in the success probability

$$\| \sin(\theta + 2k\theta) \|^2$$

- We can choose the number of iterations *k* approximately $\pi/(4\theta) \approx \sqrt{N}$ to get ”good” answers with a high success probability.

Optimality of Grover search

- Grover search can search List L of size N by calling the oracle $O(\sqrt{N})$ times

- It is proven that no quantum algorithm can perform this task by calling the oracle fewer times than $O(\sqrt{N})$.

- If you are interested in the proof,
  see ”Nielsen & Chuang Quantum Computation and Quantum Information”
  Section 6.6 Optimality of the search algorithm

Summary

- Grover search is a quantum search algorithm.
  - Call the oracle only $O(\sqrt{N})$ times while classical computers need to call $O(N)$.
  - Quadratic speed up, not exponential.
- Structure of Grover search and the details of each operator.
  1. Initialization
  2. Oracle operator
  3. Diffusion operator
     Repeat 2 and 3 $O(\sqrt{N})$ times
- How to create quantum circuits for each operator.
  - Circuits for initialization, the oracle operator, and the diffusion operator.
  - Qiskit implementation
- How Grover search works
  - Addition of probability amplitudes
  - Rotations of vectors from the geometric view.
- Optimality of Grover search