# COT 5600 Quantum Computing

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## COT 5600 Quantum Computing

- I. Linear algebra
- II. Postulates of quantum mechanics
- III. Quantum circuits
- IV. Elementary quantum algorithms
- V. Quantum Fourier transform and phase estimation
- VI. Shor's factoring algorithm
- VII. Grover's search algorithm
- VIII. ...

Linear algebra

Part I

## Complex numbers

A complex number  $z\in\mathbb{C}$  can be written as the sum of its real and imaginary parts

$$z = a + bi$$
  $a, b \in \mathbb{R}$ 

The complex conjugate  $\bar{z}$  or  $z^*$  is

$$\bar{z} = a - bi$$

The absolute value |z| is

$$|z| = \sqrt{z\bar{z}} = \sqrt{a^2 + b^2}$$

Euler's formula

$$e^{i\theta} = \cos(\theta) + i\sin(\theta), \quad \theta \in \mathbb{R}$$

read parts I and II of Chapter 1 of the book "Visual Complex Analysis" by Needham

http://people.math.sc.edu/girardi/m7034/book/VisualComplexAnalysis-Needham.pdf

## Complex vector space of dimension d

I won't give a formal definition of a vector space.

I'll explain the concepts of vector addition, scalar multiplication, linear independence, basis etc. informally using examples.

Every complex vector space of dimension d is isomorphic to the vector space  $\mathbb{C}^d$ .

We choose column vectors to represent the elements of  $\mathbb{C}^d$ .

#### Dirac notation - Kets

In the Dirac notation, vectors of a vector space are called ket vector (or kets) and denoted by

 $|v\rangle$ 

#### Dirac notation - Kets

In quantum computing, the vector spaces  $\mathbb{C}^{2^n}$  are most common. In the computational basis, the  $2^n$  basis vectors are labelled by the binary strings of length n

$$|00\dots00\rangle = \begin{pmatrix} 1\\0\\0\\\vdots\\0\\0 \end{pmatrix}, \quad |00\dots01\rangle = \begin{pmatrix} 0\\1\\0\\\vdots\\0\\0 \end{pmatrix}, \quad \dots$$

$$|11\dots 10
angle = \left(egin{array}{c} 0 \ 0 \ 0 \ dots \ 1 \ 0 \end{array}
ight), \quad |11\dots 11
angle = \left(egin{array}{c} 0 \ 0 \ 0 \ dots \ 0 \ dots \ 0 \ 1 \end{array}
ight)$$

#### Example

In  $\mathbb{C}^4$ , the ket vector

$$\sqrt{rac{2}{3}}|01
angle+rac{i}{\sqrt{3}}|11
angle=\sqrt{rac{2}{3}}|0
angle\otimes|1
angle+rac{i}{\sqrt{3}}|1
angle\otimes1
angle$$

in Dirac notation can be alternatively written as the column vector

$$\left(\begin{array}{c}0\\\sqrt{\frac{2}{3}}\\0\\\frac{i}{\sqrt{3}}\end{array}\right)$$

I will define the tensor product  $\otimes$  in more detail later

#### Inner product

An inner product on  $\mathcal{H}$  is a function

$$\langle \cdot, \cdot \rangle : \left\{ \begin{array}{ll} \mathcal{H} \times \mathcal{H} & \rightarrow & \mathbb{C} \\ (v, w) & \mapsto & \langle v, w \rangle \end{array} \right.$$

having the following properties:

▶ Linearity in the second argument

$$\langle v, \sum_{i} \lambda_{i} w_{i} \rangle = \sum_{i} \lambda_{i} \langle v, w_{i} \rangle$$

Conjugate-commutativity

$$\langle v, w \rangle = \langle w, v \rangle^*$$

► Non-negativity

$$\langle v, v \rangle \geq 0$$

with equality if and only if v = 0.

## Dot product

A familiar example of an inner product is the dot product on  $\mathbb{C}^d$  for column vectors.

The dot product of v with w is written  $v \cdot w$  and is defined as

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{pmatrix} \cdot \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{pmatrix} = (v_1^* \ v_2^* \ \dots \ v_d^*) \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{pmatrix} = \sum_{i=1}^d v_i^* w_i$$



A Hilbert space  $\ensuremath{\mathcal{H}}$  is a vector space endowed with an inner product.

## Dual Hilbert space $\mathcal{H}^*$

 $\mathcal{H}^*$  is defined to be the set of linear maps  $\mathcal{H} \to \mathbb{C}$ .

It turns out that  $\mathcal{H}^*$  is a Hilbert space that is isomorphic to  $\mathcal{H}$ .  $\mathcal{H}^*$  is called the dual of  $\mathcal{H}$  and its elements are called bra vectors.

We denote the elements of  $\mathcal{H}^*$  by  $\langle \chi |$ , where the action of  $\langle \chi |$  is:

$$\langle \chi | : | \psi \rangle \mapsto \langle \chi | \psi \rangle \in \mathbb{C}$$

Here  $\langle \chi | \psi \rangle$  is the inner product of the vector  $| \chi \rangle \in \mathcal{H}$  with the vector  $| \psi \rangle \in \mathcal{H}$ .

The bra vector  $\langle \chi |$  is called the dual of the ket vector  $|\chi \rangle$ .

In terms of matrix representation, the bra vector  $\langle \chi |$  is obtained from the ket vector  $|\chi \rangle$  by taking the corresponding row vector and taking the complex conjugate of every element (Hermitian conjugate)

#### Dirac notation

bra	$\langle \chi  $	row vector, Hermitian conjugate of $ \chi  angle$
ket	$ \psi  angle$	column vector
bra(c)ket	$\langle \chi   \psi \rangle$	complex number, dot product of $ \chi\rangle$ and $ \psi\rangle$

## Orthogonal

Two vectors  $|\chi\rangle$  and  $|\psi\rangle$  are said to be orthogonal if their inner product  $\langle\chi|\psi\rangle$  is equal to zero.

#### Norm

The norm of  $|\psi\rangle$ , denoted by  $|||\psi\rangle||$ , is the square root of the inner product of  $|\psi\rangle$  with itself, that is,

$$\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle}$$

The quantity  $||\psi\rangle|$  is called the Euclidean norm or  $\ell_2$  norm of  $|\psi\rangle$ .

A vector is called a unit vector if it has norm 1.

A set of unit vectors that are mutually orthogonal is called an orthonormal set.

#### Orthonormal basis

Let  $\mathcal{H}$  be a Hilbert space of dimension d.

A set of d vectors  $B=\{|b_i\rangle\}\subseteq \mathcal{H}$  is called an orthonormal basis for  $\mathcal{H}$  if

$$\langle b_i|b_j\rangle=\delta_{i,j}\quad \forall i,j=1,\ldots,d$$

and every  $|\psi\rangle \in \mathcal{H}$  can be written as

$$|\psi\rangle = \sum_{i=1}^d \alpha_i |b_i\rangle$$

for some  $\alpha_i \in \mathbb{C}$ .

The values  $\alpha_i$  satisfy  $\alpha_i = \langle b_i | \psi \rangle$ , and are called the coefficients of  $|\psi\rangle$  with respect to the basis  $\{|b_i\rangle\}$ .

## Orthonormal basis for $\mathcal{H}^*$

Let  $\{|b_i\rangle\}$  be an orthonormal basis for  $\mathcal{H}$ .

Then,  $\{\langle b_i|\}$  is an orthonormal basis for  $\mathcal{H}^*$  called the dual basis.

A linear operator on a vector space  $\mathcal H$  is a linear transformation  $\mathcal T:\mathcal H\to\mathcal H$  of the vector space to itself.

## Outer product

Inner product of  $|\psi\rangle$  and  $|\varphi\rangle$ 

$$\langle \psi | \varphi \rangle$$

Outer product of  $|\psi\rangle$  and  $|\varphi\rangle$ 

$$|\psi\rangle\langle\varphi|$$

## Outer product

The meaning of such an outer product  $|\psi\rangle\langle\varphi|$  is that it is a linear operator, which acts as follows:

$$\begin{aligned} \big( |\psi\rangle\langle\varphi| \big) |\gamma\rangle &= |\psi\rangle \big( \langle\varphi|\gamma\rangle \big) \\ &= \big( \langle\varphi|\gamma\rangle \big) |\psi\rangle \end{aligned}$$

The outer product of a vector  $|\psi\rangle$  with itself is written  $|\psi\rangle\langle\psi|$  and defines a linerar operator that acts as follows

$$|\psi\rangle\langle\psi||\varphi\rangle = \langle\psi|\varphi\rangle|\psi\rangle$$

This operator projects a vector  $|\varphi\rangle$  in  $\mathcal H$  onto the 1-dimensional subspace of  $\mathcal H$  spanned by  $|\psi\rangle$ 

Let  $B = \{|b_i\rangle\}$  be an orthonormal basis for  $\mathcal{H}$ . Then every linear operator  $\mathcal{T}$  on  $\mathcal{H}$  can be written as

$$T = \sum_{i,j} T_{i,j} |b_i\rangle\langle b_j|$$

where  $T_{i,j} = \langle b_i | T | b_j \rangle$ .

The set of all linear operators on  $\mathcal{H}$  forms a new complex vector space  $\mathcal{L}(\mathcal{H})$ .

All possible outer products of pairs of basis vectors from B, that is,  $|b_i\rangle\langle b_i|$  are basis vectors for  $\mathcal{L}(\mathcal{H})$ .

The action of T is then

$$T|\psi\rangle = \sum_{i,j} T_{i,j} \langle b_j | \psi \rangle | b_i \rangle = \sum_{i,j} T_{i,j} \alpha_j | b_i \rangle$$

where  $\alpha_j = \langle b_j | \psi \rangle$  are the coefficient of  $| \psi \rangle$  with respect to the ONB  $\{ |b_j \rangle \}$ .

In terms of matrix representation of T,  $T_{i,j}$  is the matrix entry in the ith row and jth column.

## Adjoint operator

Suppose T is an operator on  $\mathcal{H}$ . Then the adjoint of T, denoted  $T^{\dagger}$ , is defined as the linear operator on  $\mathcal{H}^*$  that satisfies

$$\left( \langle \psi | T^{\dagger} | \varphi \rangle \right)^* = \langle \varphi | T | \psi \rangle$$

for all  $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$ .

The matrix for  $T^{\dagger}$  is the complex conjugate transpose (also called Hermitian conjugate or adjoint) of the matrix for T.

## Unitary operators

An operator U is called unitary if

$$U^{\dagger} = U^{-1},$$

where  $U^{-1}$  is the inverse of U.

Note that  $U^{\dagger} = U^{-1}$  implies  $U^{\dagger}U = UU^{\dagger} = I$ .

The unitary operators preserve inner products between vectors, and in particular preserve the norm of vectors.

## Hermitian operators

An operator  ${\mathcal T}$  is called Hermitian (or self-adjoint) if

$$T^{\dagger}=T$$
.

## Projector

An operator P is called a projector if  $P^2 = P$ .

A projector P that also satisfies  $P^{\dagger}=P$  is called an orthogonal projector.

# Eigenvector and eigenvalue

A vector  $|\psi\rangle$  is called an eigenvector of an operator T if

$$T|\psi\rangle = c|\psi\rangle$$

for some scalar  $c \in \mathbb{C}$ .

The scalar c is called the eigenvalue of T corresponding to the eigenvector  $|\psi\rangle$ .

# Eigenvalues of Hermitian operators

If 
$$T = T^{\dagger}$$
 and if  $T|\psi\rangle = \lambda |\psi\rangle$  then  $\lambda \in \mathbb{R}$ .

In other words, the eigenvalues of a Hermitian operator are real.

#### Trace

The trace of an operator A acting on a d-dimensional Hilbert space  $\mathcal H$  is

$$\operatorname{Tr}(A) = \sum_{i=1}^d \langle b_i | T | b_i \rangle,$$

where  $\{|b_i\rangle\}$  is any orthonormal basis for  $\mathcal{H}$ .

## Normal opertors

An operator T is called normal if

$$AA^{\dagger} = A^{\dagger}A = I$$
.

Notice that unitary and Hermitian opertors are normal.

# Spectral theorm / diagonalization

For every normal operator T acting on a d-dimensional Hilbert space  $\mathcal{H}$ , there is an orthnormal basis of  $\mathcal{H}$  consisting of eigenvectors  $|\psi_i\rangle$  of T.

Note that T is diagonal in its own eigenbasis:

$$T = \sum_{i=1}^{d} \lambda_i |\psi_i\rangle\langle\psi_i|,$$

where  $\lambda_i$  is the corresponding eigenvalue to the eigenvector  $|\psi\rangle$ .

We refer to the above decomposition as the spectral decomposition of  $\mathcal{T}$ . The set of eigenvalues is called the spectrum of  $\mathcal{T}$ .

https://en.wikipedia.org/wiki/Spectral\_theorem

Diagonizable matrices do not necessarily admit an ONB https://en.wikipedia.org/wiki/Diagonalizable\_matrix

# Spectral theorem / diagonalization

For every normal matrix T acting on  $\mathbb{C}^d$ , there exists a unitary matrix U and a diagonal matrix  $\Lambda$  such that

$$T = U\Lambda U^{\dagger}$$
.

The eigenvalues of T are the entries  $\lambda_i$  of the diagonal matrix

$$\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$$

The corresponding eigenvectors of T are the columns of  $|\psi_i\rangle$  of the unitary matrix

$$U = \sum_{i=1}^{d} |\psi_i\rangle\langle i|.$$

# Simultaneous diagonalization

Let  $\{T^{(1)}, \dots, T^{(n)}\}$  be a collection of n normal operators acting on  $\mathbb{C}^d$  that commute with each other, that is,

$$T^{(k)}T^{(\ell)} = T^{(\ell)}T^{(k)}$$

for all  $k, \ell \in \{1, \ldots, n\}$ .

Then, there exist a simulateneous eigenvector basis  $\{|\psi_1\rangle, \dots, |\psi_d\rangle\}$  for all operators such that

$$T^{(k)}|\psi_i\rangle = \lambda_i^{(k)}|\psi_i\rangle.$$

for all  $k \in \{1, \ldots, n\}$  and all  $i \in \{1, \ldots, d\}$ .

## **Functions of Operators**

Let  $f: \mathbb{C} \to \mathbb{C}$  an arbitrary function and

$$T = \sum_{i=1}^{d} \lambda_i |\psi\rangle\langle\psi_i| = U \Lambda U^{\dagger}$$

be the diagonalization of the normal operator T.

Then, we define

$$f(T) := \sum_{i=1}^d f(\lambda_i) |\psi_i\rangle \langle \psi_i| = U f(\Lambda) U^{\dagger}$$

where

$$f(\Lambda) = \operatorname{diag}(f(\lambda_1), \dots, f(\lambda_d)).$$

## Tensor product

The tensor product is a way of combining vector spaces https://en.wikipedia.org/wiki/Tensor\_product

Suppose  $\mathcal{H}_1$  and  $\mathcal{H}_2$  are Hilbert spaces of dimensions  $d_1$  and  $d_2$ .

Then, the new tensor product space  $\mathcal{H}_1 \otimes \mathcal{H}_2$  is a new larger Hilbert space of dimension  $d_1 \cdot d_2$ .

Suppose

$$\{|b_i\rangle \text{ and } \{|c_j\rangle\}$$

are orthonormal bases for  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , respectively.

Then,

$$\{|b_i\rangle\otimes|c_j\rangle\}$$

is an orthonormal basis for  $\mathcal{H}_1 \otimes \mathcal{H}_2$ .

## Properties of the tensor product

The tensor product of two vectors  $|\psi_1\rangle \in \mathcal{H}_1$  and  $|\psi_2\rangle \in \mathcal{H}_2$  is a vector in  $\mathcal{H}_1 \otimes \mathcal{H}_2$ , and is written as  $|\psi_1\rangle \otimes |\psi_2\rangle$ .

The tensor product is characterized by the following axioms:

1. for any  $c \in \mathbb{C}$ ,  $|\psi_1\rangle \in \mathcal{H}_1$ , and  $|\psi_2\rangle \in \mathcal{H}_2$ ,

$$c(|\psi_1\rangle \otimes |\psi_2\rangle) = (c|\psi_1\rangle) \otimes |\psi_2\rangle = |\psi_1\rangle \otimes (c|\psi_2\rangle)$$

2. for any  $|\psi_1\rangle, |\varphi_1\rangle \in \mathcal{H}_1$ , and  $|\psi_2\rangle \in \mathcal{H}_2$ ,

$$(|\psi_1\rangle + |\varphi_1\rangle) \otimes |\psi_2\rangle = (|\psi_1\rangle \otimes |\psi_2\rangle + |\varphi_1\rangle \otimes |\psi_2\rangle$$

3. for any  $|\psi_1\rangle \in \mathcal{H}_1$ , and  $|\psi_2\rangle, |\varphi_2\rangle \in \mathcal{H}_2$ ,

$$|\psi_1\rangle \otimes (|\psi_2\rangle + |\varphi_2\rangle) = |\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1\rangle \otimes |\varphi_2\rangle$$

# Properties of tensor product

Suppose  $A \in \mathcal{L}(\mathcal{H}_1)$  and  $B \in \mathcal{L}(\mathcal{H}_2)$ , respectively.

Then  $A \otimes B \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  is defined by

$$(A \otimes B)(|\psi_1\rangle \otimes |\psi_2\rangle) = A|\psi_1\rangle \otimes B|\psi_2\rangle$$

for all  $|\psi_1\rangle \in \mathcal{H}_1$ ,  $|\psi_2\rangle \in \mathcal{H}_2$ .

This definition extends linearly over the elements of  $\mathcal{H}_1 \otimes \mathcal{H}_2$ 

$$(A \otimes B) (\sum_{ij} \alpha_{ij} |b_i\rangle \otimes |b_j\rangle) = \sum_{ij} \alpha_{ij} A |b_i\rangle \otimes B |b_j\rangle.$$

#### Norm for matrices

Let  $X \in \mathcal{L}(\mathcal{H})$ .

The norm ||X|| is defined as

$$\|X\| = \max_{|\psi\rangle \in \mathcal{H}} \frac{\|X|\psi\rangle\|}{\||\psi\rangle\|}$$
.

Note that there are other norms for matrices: https://en.wikipedia.org/wiki/Matrix\_norm

The above matrix norm is the norm induced by the  $\ell_2$  vector norm.

## Part II

Postulates of quantum mechanics

# The state of a quantum system

#### State Space Postulate

The state of a system is described by a unit vector in a Hilbert space  $\mathcal{H}$ .

#### Time-Evolution of a Closed System

#### **Evolution Postulate**

The time-evolution of the state of a closed quantum system is described by a unitary operator.

That is, for any evolution of the closed system there exsists a unitary operator U such that if the initial state of the system was  $|\psi_1\rangle$ , then after the evolution the state of the system will be

$$|\psi_2\rangle = U|\psi_1\rangle$$
.

## Composite Systems

#### Composition of Systems Postulate

When two physical systems are treated as one combined system, the state space of the physical system is the tensor product space  $\mathcal{H}_1 \otimes \mathcal{H}_2$  of the state spaces  $\mathcal{H}_1, \mathcal{H}_2$  of the component subsystems.

If the first subsystem is in the state  $|\psi_1\rangle$  and the second system in the state  $|\psi_2\rangle$ , then the state of the combined system is

$$|\psi_1\rangle\otimes|\psi_2\rangle$$
.

#### Measurement

#### Measurement Postulate

For a given ONB  $B=\{|\varphi_i\rangle\}$  of a state space  $\mathcal{H}$ , it is possible to perform a Von Neuman measurement on system  $\mathcal{H}$  with respect to B that, given a state

$$|\psi\rangle = \sum_{i} \alpha_{i} |\varphi_{i}\rangle$$

outputs a label i with probability

$$\Pr(i) = |\alpha_i|^2$$

and leaves the system in the state

$$|\varphi_i\rangle$$
.

#### Measurement - continued

#### Measurement Postulate

Furthermore, given a state

$$|\psi\rangle = \sum_{i} \alpha_{i} |\varphi_{i}\rangle |\gamma_{i}\rangle$$

from a bipartite state space  $\mathcal{H}\otimes\mathcal{H}'$ , then performing a Von Neumann measurement on system  $\mathcal{H}$  will yield outcome i with probability

$$Pr(i) = |\alpha_i|^2$$

and leave the bipartite system in state

$$|\varphi_i\rangle|\gamma_i\rangle$$
.

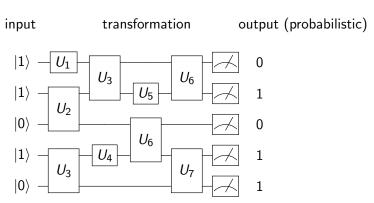
Note that the  $|\gamma_i\rangle$  have unit norm but are not necessarily orthogonal.

Quantum circuits

Part III

#### Quantum circuit model

Quantum circuits are generalizations of Boolean circuits



#### Classical bit

Classical bit (bit):  $\mathbb{B} := \{0, 1\}$ 

- ▶ Basis state: either 0 or 1
- lacktriangle General state: a probability distribution  $p=(p_0,p_1)$  on  $\mathbb B$

# Classical register

Classical register: 
$$\mathbb{B}^n := \underbrace{\mathbb{B} \times \mathbb{B} \times \ldots \times \mathbb{B}}_{n}$$

- ▶ Basis state: a binary string  $x \in \mathbb{B}^n$
- ▶ General state: a probability distribution  $p = (p_x : x \in \mathbb{B}^n)$  on  $\mathbb{B}^n$  (written as a column vector)

Remark: Note that p is a vector with positive entries that is normalized with respect to the  $\ell_1$ -norm (the sum of the absolute values of the entries)

#### Classical transformation

Transformations on the classical register  $\ensuremath{\mathbb{B}}$  are described by stochastic matrices

Stochastic matrices preserve the  $\ell_1$ -norm, i.e., probability distributions are mapped on probability distributions

Let p be the state of the register. The state after the transformation P is given by the matrix-vector-product

#### Qubit

Quantum bit (qubit): two-dimensional complex Hilbert space  $\mathbb{C}^2$ 

Computational basis states (classical states):

$$|0\rangle := \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \qquad \text{and} \qquad |1\rangle := \left( \begin{array}{c} 0 \\ 1 \end{array} \right)$$

General states: superpositions

$$|\psi\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \alpha_0 |0\rangle + \alpha_1 |1\rangle, \quad |\alpha_0|^2 + |\alpha_1|^2 = 1$$

the coefficients  $\alpha_0, \alpha_1 \in \mathbb{C}$  are called probability amplitudes

### Quantum register

Quantum register:  $2^n$ -dimensional complex Hilbert space  $(\mathbb{C}^2)^{\otimes n}$  with tensor product structure

$$(\mathbb{C}^2)^{\otimes n} := \underbrace{\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{n}$$

Computational basis states (classical states):

$$|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle, \quad x \in \mathbb{B}^n$$

► General state:

$$|\psi\rangle = \sum_{x \in \mathbb{T}^n} \alpha_x |x\rangle, \quad \sum_{x \in \mathbb{T}^n} |\alpha_x|^2 = 1$$

Remark: Note that  $|\psi\rangle$  is a column vector (ket) that is normalized with respect to the  $\ell_2$ -norm (Euclidean norm)

#### Quantum transformations

Transformations on the quantum register  $\mathcal{H}:=(\mathbb{C}^2)^{\otimes n}$  are described by unitary matrices  $U\in\mathcal{U}(\mathcal{H})$ 

Unitary matrices preserve the  $\ell_2$ -norm

Let  $|\psi\rangle\in\mathcal{H}$  be the state of the quantum register; the state after the transformation U is given by the matrix-vector product

$$U|\psi\rangle$$

#### Quantum circuit

Each transformations U has to be implemented by a quantum circuit, i.e., a sequence of elementary gates

 $\label{eq:Quantum circuit model} \textbf{Quantum mechanics} + \textbf{Notion of} \\ \textbf{complexity}$ 

# Single qubit gate on two qubits

single-qubit gate 
$$\it U$$
 on first qubit

action on basis states of 
$$\mathbb{C}^2 \otimes \mathbb{C}^2$$
 
$$\begin{vmatrix} |0\rangle \otimes |0\rangle & \mapsto & (\textcolor{red}{U}|0\rangle) \otimes |0\rangle \\ |0\rangle \otimes |1\rangle & \mapsto & (\textcolor{red}{U}|0\rangle) \otimes |1\rangle \\ |1\rangle \otimes |0\rangle & \mapsto & (\textcolor{red}{U}|1\rangle) \otimes |0\rangle \\ |1\rangle \otimes |1\rangle & \mapsto & (\textcolor{red}{U}|1\rangle) \otimes |1\rangle \\ \end{aligned}$$

corresponding matrix

$$U \otimes I = \left(\begin{array}{c|cc|c} u_{00} \cdot I & u_{01} \cdot I \\ \hline u_{10} \cdot I & u_{11} \cdot I \end{array}\right) = \left(\begin{array}{ccc|c} u_{00} & 0 & u_{01} & 0 \\ 0 & u_{00} & 0 & u_{01} \\ u_{10} & 0 & u_{11} & 0 \\ 0 & u_{10} & 0 & u_{11} \end{array}\right)$$

# Single qubit gate on two qubits

single-qubit gate U on second qubit

$$-U$$

action on basis states of 
$$\mathbb{C}^2 \otimes \mathbb{C}^2$$
  $\begin{vmatrix} |0\rangle \otimes |1\rangle & \mapsto & |0\rangle \otimes U|1\rangle \\ |1\rangle \otimes |0\rangle & \mapsto & |1\rangle \otimes U|0\rangle \end{vmatrix}$ 

$$\begin{array}{ccc} |0\rangle \otimes |1\rangle & \mapsto & |0\rangle \otimes U|1\rangle \\ |1\rangle \otimes |0\rangle & \mapsto & |1\rangle \otimes U|0\rangle \\ |1\rangle \otimes |1\rangle & \mapsto & |1\rangle \otimes U|1\rangle \end{array}$$

 $|0\rangle \otimes |0\rangle \mapsto |0\rangle \otimes U|0\rangle$ 

corresponding matrix

$$I \otimes U = \left(\begin{array}{c|cc|c} 1 \cdot U & 0 \cdot U \\ \hline 0 \cdot U & 1 \cdot U \end{array}\right) = \left(\begin{array}{ccc|c} u_{00} & u_{01} & 0 & 0 \\ u_{10} & u_{11} & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{array}\right)$$

# Controlled-NOT gate

control: first qubit; target: second qubit



action on basis states of  $\mathbb{C}^2 \otimes \mathbb{C}^2$ 

$$|c\rangle\otimes|t\rangle\mapsto|c\rangle\otimes|c\oplus t\rangle$$

corresponding matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = |0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes X$$

where  $I_2 = |0\rangle\langle 0| + |1\rangle\langle 1|$  and  $X = |0\rangle\langle 1| + |1\rangle\langle 0|$ 

# Controlled U gate

control: qubit; target: m-qubit register



let U be a unitary acting on the m-qubit register action on basis states of  $\mathbb{C}^2\otimes (\mathbb{C}^2)^{\otimes m}$ 

$$|c\rangle\otimes|t\rangle\mapsto|c\rangle\otimes U^c|t\rangle$$
 where  $b\in\mathbb{B},t\in\mathbb{B}^m$ 

corresponding matrix

$$\left(\begin{array}{c|c} I & 0 \\ \hline 0 & U \end{array}\right) = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$$

#### Toffoli gate

control: first and second qubits; target: third qubit



action on basis states of  $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ 

$$|c_1\rangle\otimes|c_2\rangle\otimes|t\rangle\mapsto|c_1\rangle\otimes|c_2\rangle\otimes|(c_1\wedge c_2)\oplus t\rangle$$

corresponding matrix

corresponding matrix 
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = (I_4 - |11\rangle\langle11|) \otimes I_2 + |11\rangle\langle11| \otimes X$$
 https://en.wikipedia.org/wiki/Toffoli\_gate

# Reversible computing & Fredkin gate

Reversible computing

https://en.wikipedia.org/wiki/Reversible\_computing

The so-called Fredkin gate is universal for reversible computing.

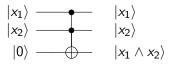
https://en.wikipedia.org/wiki/Fredkin\_gate

# Simulating irreversible gates with Toffoli gate

The classical AND gate is irreversible because if the output is 0 then we cannot determine which of the three possible pairs was the actual input

$x_1$	<i>X</i> <sub>2</sub>	$x_1 \wedge x_2$
0	0	0
0	1	0
1	0	0
1	1	1

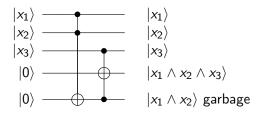
But it is easy to simulate the AND gate with one Toffoli gate



# Problem of garbage

To simulate irreversible circuits with Toffoli gates, we keep the input and intermediary results to make everything reversible

Consider the function  $y = x_1 \land x_2 \land x_3$ 

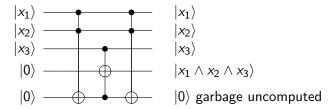


It is important to not leave any garbage; otherwise, we could not make use of quantum parallelism and constructive interference effects

## Reversible garbage removal

It is always possible to reversibly remove (uncompute) the garbage

In the case  $y = x_1 \wedge x_2 \wedge x_3$ , this can be done with the circuit



# Simulating irreversible circuits with Toffoli gates

Let  $f: \{0,1\}^n \to \{0,1\}$  be any boolean function

Assume this function can be computed classically using only t classical elementary gates such as AND, OR, NAND

We can implement a unitary  $U_f$  on  $(\mathbb{C}^2)^{\otimes n}\otimes \mathbb{C}^2\otimes (\mathbb{C}^2)^{\otimes w}$  such that

$$U_f(|x\rangle_{\mathrm{in}}\otimes|y\rangle_{\mathrm{out}}\otimes|0\rangle_{\mathrm{work}}^{\otimes w})=|x\rangle\otimes|y\oplus f(x)\rangle\otimes|0\rangle^{\otimes w}$$

 $U_f$  is built from polynomially many in t Toffoli gates and the size w of the workspace register is polynomial in t

During the computation the qubits of the workspace register are changed, but at the end they reversibly reset to  $|0\rangle^{\otimes w}$ 

## Universal gate set – exact implementation

Each unitary  $U \in \mathcal{U}(\mathcal{H})$  can be implemented exactly by quantum circuits using only:

- CNOT gates (acting on adjacent qubits)
- ► arbitrary single qubit gates

Elementary quantum gates for quantum computation Barenco et al.

https://arxiv.org/abs/quant-ph/9503016

## Gate complexity of unitaries – exact implementation

The gate complexity  $\kappa(U)$  of a unitary  $U \in \mathcal{U}(\mathcal{H})$  is minimal number of elementary gates needed to implement U

For example, quantum Fourier Transform has complexity  $O(n^2)$ 

⇒ Shor's factorization algorithm

## Universal gate set – approximate implementation

For each  $\epsilon \in (0,1)$  and each unitary  $U \in \mathcal{U}(\mathcal{H})$ , there is a unitary V such that

$$\|U-V\| \leq \epsilon \quad ext{where} \quad \|U-V\| = \sup_{|\psi
angle} \|(U-V)|\psi
angle\|$$

and V is implemented by quantum circuits using only:

- CNOT gates (acting on adjacent qubits)
- ► the single qubit gates

$$H=rac{1}{\sqrt{2}}\left(egin{array}{cc} 1 & 1 \ 1 & -1 \end{array}
ight) \quad R( heta)=\left(egin{array}{cc} 1 & 0 \ 0 & e^{i heta} \end{array}
ight)\,, \quad {
m with}\,\, heta=rac{\pi}{4}$$

There are other universal gate sets

# Gate complexity of unitaries – approximate implementation

The gate complexity  $\kappa_{\epsilon}(U)$  of a unitary U is the minimal number of gates (from a universal gate set) need to implement a unitary V with  $\|U-V\| \leq \epsilon$ 

The Solovay-Kitaev theorem implies that

$$\kappa_{\epsilon}(U) = O\left(\kappa(U) \cdot \log^{c}\left(\kappa(U)/\epsilon\right)\right)$$

for some small constant c

The Solovay-Kitaev algorithm, Dawson and Nielsen, https://arxiv.org/abs/quant-ph/0505030

## Gate complexity of unitaries

Counting arguments show that most n-qubit unitaries have gate complexity exponential in n.

#### Quantum measurement

A general measurement is described by a collection  $P_0, \ldots, P_{m-1}$  of orthogonal projectors such that

$$\sum_{i=0}^{m-1} P_i = I_{\mathcal{H}}$$
 where  ${\mathcal{H}}$  denotes the identity on  ${\mathcal{H}}$ 

Let  $|\psi\rangle$  be the state of the quantum register. The probability of obtaining the outcome i is given by

$$\Pr(i) = \|P_i|\psi\rangle\|^2$$

The post-measurement state (collapse of the wavefunction) is

$$\frac{P_i|\psi\rangle}{\|P_i|\psi\rangle\|}$$

#### Elementary quantum measurements

A measurement has to be realized by first applying a suitable quantum circuit followed by an elementary measurement

An elementary measurement on the n-qubit quantum register  $\mathcal{H}$  consists of measuring the first (w.l.o.g.) m qubits ( $m \leq n$ ) with respect to the computational basis

The  $2^m$  orthogonal projectors  $P_b$  are labeled by m-bit strings  $b \in \mathbb{B}^m$  and are defined by

$$P_b = |b_1\rangle\langle b_1| \otimes |b_2\rangle\langle b_2| \otimes \cdots \otimes |b_m\rangle\langle b_m| \otimes I_{2^{n-m}}$$

The probability of obtaining outcome b is given by

$$\Pr(b) = \|P_b|\psi\rangle\|^2 = \sum_{x_{m+1},...,x_n \in \mathbb{B}} |\alpha_{b_1,...,b_m,x_{m+1},...,x_n}|^2$$

### Structure of quantum algorithms

#### A quantum algorithm consists of

- ▶ preparing the initial state  $|x\rangle$  with  $x \in \mathbb{B}^n$ ,
- ► applying a quantum circuit of polynomially many in *n* gates from some universal gate set, and
- performing an elementary measurement

These steps are repeated polynomially many times to collect enough samples and followed by classical post-processing  $\Longrightarrow$  solution of the problem

### Hadamard test

The probabilities of obtaining the outcomes 0 and 1 are:

$$\mathsf{Pr}(0) = \frac{1}{2} \left( 1 + \mathrm{Re} \langle \psi | U | \psi \rangle \right) \qquad \mathsf{Pr}(1) = \frac{1}{2} \left( 1 - \mathrm{Re} \langle \psi | U | \psi \rangle \right)$$

# Hadamard test

$$|0\rangle$$
  $H$   $H$   $|\psi\rangle$   $U$ 

$$|0\rangle \otimes |\psi\rangle$$

$$\mapsto \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes |\psi\rangle$$

$$= \frac{1}{\sqrt{2}} |0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes |\psi\rangle$$

$$\mapsto \frac{1}{\sqrt{2}} |0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes U|\psi\rangle$$

$$\mapsto \frac{1}{2} (|0\rangle + |1\rangle) \otimes |\psi\rangle + \frac{1}{2} (|0\rangle - |1\rangle) \otimes U|\psi\rangle$$

$$= \frac{1}{2} |0\rangle \otimes (|\psi\rangle + U|\psi\rangle) + \frac{1}{2} |1\rangle \otimes (|\psi\rangle - U|\psi\rangle)$$

$$=: |\Phi\rangle$$

### Hadamard test

$$\begin{aligned} & \Pr(0) \\ &= \|P|\Phi\rangle\|^2 \quad \text{with} \quad P = |0\rangle\langle 0| \otimes I \\ &= \|\left(|0\rangle\langle 0| \otimes I\right) \left(\frac{1}{2}|0\rangle \otimes (|\psi\rangle + U|\psi\rangle) + \frac{1}{2}|1\rangle \otimes (|\psi\rangle - U|\psi\rangle)\right)\|^2 \\ &= \|\frac{1}{2}|0\rangle \otimes (|\psi\rangle + U|\psi\rangle)\|^2 \\ &= \frac{1}{4}\||0\rangle\|^2 \cdot \||\psi\rangle + U|\psi\rangle\|^2 \\ &= \frac{1}{4}\left(\langle \psi| + \langle \psi|U^{\dagger} \rangle \left(|\psi\rangle + U|\psi\rangle\right) \\ &= \frac{1}{4}\left(\langle \psi|\psi\rangle + \langle \psi|U|\psi\rangle + \langle \psi|U^{\dagger}|\psi\rangle + \langle \psi|U^{\dagger}U|\psi\rangle\right) \\ &= \frac{1}{4}\left(2 + \langle \psi|U|\psi\rangle + \overline{\langle \psi|U|\psi\rangle}\right) \\ &= \frac{1}{2}\left(1 + \operatorname{Re}\langle \psi|U|\psi\rangle\right) \end{aligned}$$

## Hadamard test – Figure it out yourself

How can you estimate the imaginary part of  $\langle \psi | U | \psi \rangle$ ?

Hint: Add a simple gate on the control register before the measurement.

## SWAP test - Figure it out yourself

Let S denote the swap gate acting on two qubits

$$S = |00\rangle\langle00| + |01\rangle\langle10| + |10\rangle\langle01| + |11\rangle\langle11|$$

Determine the matrix representation of  $\boldsymbol{S}$  with respect to the computational basis

Consider the Hadamard test where the controlled operation is

$$|0\rangle\langle 0|\otimes I_4+|1\rangle\langle 1|\otimes S$$

and the state of the target register  $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ 

Determine the probability of obtaining 0 and 1 for the cases:

- ► arbitrary  $|\psi_1\rangle$  and  $|\psi_2\rangle$ , ►  $\langle \psi_1|\psi_2\rangle = 0$  (orthogonal), and
  - $\langle \psi_1 | \psi_2 \rangle = 0$  (orthogonal), and
  - $\blacktriangleright \langle \psi_1 | \psi_2 \rangle = 1$  (the same).

# Part IV

# Elementary quantum algorithms

### Black box problems

Standard computational problem: determine a property of some input data

Example: Find the prime factors of N

Alternate model: Input is provided by a black box (or oracle)

- ▶ Query: On input x, black box returns f(x)
- ▶ Determine a property of *f* using as few queries as possible
- ► The minimum number of queries is the *query complexity*
- Example: Given a black box for  $f : \{1, 2, ..., N\} \rightarrow \{0, 1\}$ , is there some x such that f(x) = 1?
- Why black boxes?
  - Facilitates proving lower bounds
  - Can lead to algorithms for standard problems

# Black boxes for reversible/quantum computing

Black box 
$$x - f - f(x)$$
 is not reversible

Given a circuit that computes f non-reversibly, we can implement the reversible version with little overhead

Quantum version: 
$$|x\rangle$$
  $|x\rangle$   $|z\rangle$   $|z\oplus f(x)\rangle$ 

A reversible circuit is a quantum circuit

## Deutsch's problem

#### Problem

- ▶ Given: a black-box function  $f: \{0,1\} \rightarrow \{0,1\}$
- ► Task: determine whether f is constant or balanced

How many queries are needed?

- Classically: 2 queries are necessary and sufficient
- Quantumly: ?

## Toward a quantum algorithm for Deutsch's problem

Quantum black box for 
$$f: |x\rangle - |x\rangle$$

$$|z\rangle - |z \oplus f(x)\rangle$$

Compute 
$$f$$
 in superposition:  $|0\rangle$   $H$   $f$   $|0\rangle$ 

$$|0\rangle \otimes |0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle \ \mapsto \frac{1}{\sqrt{2}} (|0\rangle \otimes |f(0)\rangle + |1\rangle \otimes |f(1)\rangle)$$

Can't extract more than one bit of information about f

### Phase kickback

Quantum black box for 
$$f: |x\rangle$$

$$|z\rangle - f - |x\rangle$$

$$|z \oplus f(x)\rangle$$

Phase kickback:

$$\frac{|x\rangle}{\frac{|0\rangle-|1\rangle}{\sqrt{2}}} - \boxed{f} - \frac{(-1)^{f(x)}|x\rangle}{\frac{|0\rangle-|1\rangle}{\sqrt{2}}}$$

$$|x\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}}(|x\rangle \otimes |0\rangle - |x\rangle \otimes |1\rangle)$$

$$\mapsto \frac{1}{\sqrt{2}}(|x\rangle \otimes |f(x)\rangle - |x\rangle \otimes |1 \oplus f(x)\rangle)$$

$$= |x\rangle \otimes \frac{1}{\sqrt{2}}(|f(x)\rangle - |\overline{f(x)}\rangle)$$

$$= \underbrace{(-1)^{f(x)}}_{\text{not necessarily global}}|x\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

# Quantum algorithm for Deutsch's problem

$$\begin{split} |0\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} &\mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \\ &\mapsto \frac{(-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \\ &= (-1)^{f(0)} \frac{|0\rangle + (-1)^{f(0) \oplus f(1)}|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \\ &\mapsto (-1)^{f(0)} |f(0) \oplus f(1)\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \end{split}$$

1 quantum query vs. 2 classical queries!

### The Deutsch-Jozsa problem

#### Problem

- ▶ Given: a black-box function  $f: \{0,1\}^n \to \{0,1\}$
- Promise: f is either constant (f(x)) is independent of x or balanced (f(x)) = 0 for exactly half the values of x
- ► Task: determine whether f is constant or balanced

#### How many queries are needed?

- ▶ Classically:  $2^n/2 + 1$  queries to answer with certainty
- Quantumly: ?

### Phase kickback for a Boolean function of *n* bits

Black box function: 
$$|x_1\rangle$$
  $|x_1\rangle$   $\vdots$   $|x_n\rangle$   $|z\rangle$   $|z\oplus f(x)\rangle$ 

Phase kickback:

$$|x_1\rangle\otimes\cdots\otimes|x_n\rangle\otimes\frac{|0\rangle-|1\rangle}{\sqrt{2}}\mapsto (-1)^{f(x)}|x_1\rangle\otimes\cdots\otimes|x_n\rangle\otimes\frac{|0\rangle-|1\rangle}{\sqrt{2}}$$

# Quantum algorithm for the Deutsch-Jozsa problem

$$|0\rangle^{\otimes n} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \mapsto \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right)^{\otimes n} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$= \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$\mapsto \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

#### Hadamard transform

What do the final Hadamard gates do?

$$H|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + (-1)^{x}|1\rangle)$$
$$= \frac{1}{\sqrt{2}}\sum_{y \in \{0,1\}} (-1)^{xy}|y\rangle$$

$$H^{\otimes n}(|x_1\rangle \otimes \cdots \otimes |x_n\rangle) = \bigotimes_{i=1}^n \left(\frac{1}{\sqrt{2}} \sum_{y_i \in \{0,1\}} (-1)^{x_i y_i} |y_i\rangle\right)$$

$$= \frac{1}{\sqrt{2^n}} \sum_{y \in \{0,1\}^n} (-1)^{x \cdot y} |y\rangle$$

# Quantum D-J algorithm: Finishing up

$$\frac{1}{\sqrt{2^{n}}} \sum_{x \in \{0,1\}^{n}} (-1)^{f(x)} |x\rangle \overset{H^{\otimes n}}{\mapsto} \frac{1}{2^{n}} \sum_{x,y \in \{0,1\}^{n}} (-1)^{f(x)} (-1)^{x \cdot y} |y\rangle$$

▶ If f is constant, the amplitude of  $|y\rangle$  is

$$\pm \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{x \cdot y} = \pm \begin{cases} 1 & \text{if } y = 0 \dots 0 \\ 0 & \text{otherwise} \end{cases}$$

so we definitely measure 0...0

▶ If f is balanced, the amplitude of  $|0...0\rangle$  is

$$\sum_{x \in \{0,1\}^n} (-1)^{f(x)} = 0$$

so we measure some nonzero string

### The Deutsch-Jozsa problem: Quantum vs. classical

Above quantum algorithm uses only one query.

Need  $2^n/2 + 1$  classical queries to answer with certainty.

What about randomized algorithms? Success probability arbitrarily close to 1 with a constant number of queries.

Can we get a separation between randomized and quantum computation?

# Simon's problem

#### Problem

- ▶ Given: a black-box function  $f: \{0,1\}^n \rightarrow \{0,1\}^m$
- ▶ Promise: there is some  $s \in \{0,1\}^n$  such that f(x) = f(y) if and only if x = y or  $x = y \oplus s$
- ► Task: determine s

#### One classical strategy:

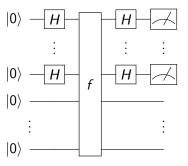
- query a random x
- repeat until we find  $x_i \neq x_j$  such that  $f(x_i) = f(x_j)$
- **output**  $x_i \oplus x_j$

By the birthday problem, this uses about  $\sqrt{2^n}$  queries.

It can be shown that this strategy is essentially optimal.

# Quantum algorithm for Simon's problem

Quantum black box: 
$$|x\rangle\otimes|y\rangle\mapsto|x\rangle\otimes|y\oplus f(x)\rangle$$
 
$$(x\in\{0,1\}^n,\ y\in\{0,1\}^m)$$



Repeat many times and post-process the measurement outcomes

# Quantum algorithm for Simon's problem: Analysis I

$$|0\rangle \stackrel{H}{\longrightarrow} H \stackrel{}{\longrightarrow} H \stackrel{}{\longrightarrow$$

# Quantum algorithm for Simon's problem: Analysis II

Recall 
$$H^{\otimes n}|x\rangle = \sum_{y \in \{0,1\}^n} (-1)^{x \cdot y} |y\rangle$$

$$H^{\otimes n}\left(\frac{|x\rangle+|x\oplus s\rangle}{\sqrt{2}}\right) = \frac{1}{\sqrt{2^{n+1}}} \sum_{y\in\{0,1\}^n} [(-1)^{x\cdot y} + (-1)^{(x\oplus s)\cdot y}]|y\rangle$$
$$= \frac{1}{\sqrt{2^{n+1}}} \sum_{y\in\{0,1\}^n} (-1)^{x\cdot y} [1 + (-1)^{s\cdot y}]|y\rangle$$

Two cases:

- if  $s \cdot y = 0 \mod 2$ ,  $1 + (-1)^{s \cdot y} = 2$
- if  $s \cdot y = 1 \mod 2$ ,  $1 + (-1)^{s \cdot y} = 0$

Measuring gives a random y orthogonal to s (i.e.,  $s \cdot y = 0$ )

# Quantum algorithm for Simon's problem: Post-processing

Measuring gives a random y orthogonal to s ( $s \cdot y = 0$ )

Repeat k times, giving vectors  $y_1, \ldots, y_k \in \{0, 1\}^n$ ; solve a system of k linear equations for  $s \in \{0, 1\}^n$ :

$$y_1 \cdot s = 0$$
,  $y_2 \cdot s = 0$ , ...,  $y_k \cdot s = 0$ 

How big should k be to give a unique (nonzero) solution?

- ▶ Clearly  $k \ge n 1$  is necessary
- ▶ It can be shown that k = O(n) suffices

O(n) quantum queries,  $O(n^3)$  quantum gates

Compare to  $\Omega(2^{n/2})$  classical queries (even for bounded error)

### Recap

We have seen several examples of quantum algorithms that outperform classical computation:

- ▶ Deutsch's problem: 1 quantum query vs. 2 classical queries
- ▶ Deutsch-Jozsa problem: 1 quantum query vs.  $2^{\Omega(n)}$  classical queries (deterministic)
- Simon's problem: O(n) quantum queries vs.  $2^{\Omega(n)}$  classical queries (randomized)

Quantum algorithms for more interesting problems build on the tools used in these examples.

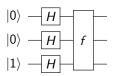
### Exercise: One-out-of-four search

Let  $f:\{0,1\}^2 \to \{0,1\}$  be a black-box function taking the value 1 on exactly one input. The goal is to find the unique  $(x_1,x_2) \in \{0,1\}^2$  such that  $f(x_1,x_2)=1$ .

- Write the truth tables of the four possible functions f.
- ▶ How many classical queries are needed to solve the problem?
- ▶ Suppose f is given as a quantum black box  $U_f$  acting as

$$|x_1,x_2,y\rangle\mapsto |x_1,x_2,y\oplus f(x_1,x_2)\rangle.$$

Determine the output of the following quantum circuit for each of the possible black-box functions f:



Show that the four possible outputs obtained in the previous part are pairwise orthogonal. What can you conclude about the quantum query complexity of one-out-of-four search?

The QFT and phase estimation

Part V

# Quantum phase estimation

#### Problem

We are given a unitary U and an eigenvector  $|\psi\rangle$  of U with unknown eigenvalue

We seek to determine its eigenphase  $\varphi \in [0,1)$  such that

$$U|\psi\rangle = e^{2\pi i \varphi}|\psi\rangle$$

More precisely, we want to obtain an estimate  $\hat{arphi}$  such that

$$\Pr\left(|\hat{\varphi} - \varphi| \le \frac{1}{2^n}\right) \ge \frac{3}{4}$$

The deviation  $|\hat{\varphi} - \varphi|$  is computed modulo 1

## Phase kick back

$$\begin{array}{c|c} |+\rangle & & \\ |\psi\rangle & - U - \end{array}$$

$$\begin{split} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\psi\rangle &= \frac{|0\rangle}{\sqrt{2}} \otimes |\psi\rangle + \frac{|1\rangle}{\sqrt{2}} \otimes |\psi\rangle \\ &\mapsto \frac{|0\rangle}{\sqrt{2}} \otimes |\psi\rangle + \frac{|1\rangle}{\sqrt{2}} \otimes U|\psi\rangle \\ &= \frac{|0\rangle}{\sqrt{2}} \otimes |\psi\rangle + \frac{|1\rangle}{\sqrt{2}} \otimes e^{2\pi i \varphi} |\psi\rangle \\ &= \frac{|0\rangle}{\sqrt{2}} \otimes |\psi\rangle + \frac{e^{2\pi i \varphi} |1\rangle}{\sqrt{2}} \otimes |\psi\rangle \\ &= \frac{|0\rangle + e^{2\pi i \varphi} |1\rangle}{\sqrt{2}} \otimes |\psi\rangle \end{split}$$

#### Phase kick back

$$\begin{array}{c} |+\rangle & - \\ |\psi\rangle & - |U| - \\ \\ \hline \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\psi\rangle \mapsto \frac{|0\rangle + e^{2\pi i \varphi} |1\rangle}{\sqrt{2}} \otimes |\psi\rangle \end{array}$$

The eigenstate  $|\psi\rangle$  in the target register emerges unchanged

⇒ It suffices to focus on the control register

The state  $|0\rangle+|1\rangle$  of the control qubit is changed to  $|0\rangle+e^{2\pi i\varphi}|1\rangle$  by phase kick back

# ${\sf Hadamard\ test\ +\ phase\ kick\ back}$

$$|0\rangle - H - H$$

$$|\psi\rangle - U$$

$$\frac{|0\rangle + e^{2\pi i \varphi}|1\rangle}{\sqrt{2}}$$

$$\begin{array}{ll} \mapsto & \frac{1}{2} \left( (|0\rangle + |1\rangle) + \mathrm{e}^{2\pi i \varphi} (|0\rangle - |1\rangle) \right) \\ \mapsto & \frac{1}{2} \left( (1 + \mathrm{e}^{2\pi i \varphi}) |0\rangle + (1 - \mathrm{e}^{2\pi i \varphi}) |1\rangle) \right) := |\varphi\rangle \end{array}$$

# Hadamard test + phase kick back

$$|arphi
angle = rac{1}{2} \left( (1 + e^{2\pi i arphi}) |0
angle + (1 - e^{2\pi i arphi}) |1
angle ) 
ight)$$

The probability of obtaining 0 is

$$Pr(0) = |||0\rangle\langle 0||\varphi\rangle||^{2}$$

$$= |\frac{1}{2}(1 + e^{2\pi i\varphi})|^{2}$$

$$= \frac{1}{4}|e^{\pi i\varphi} + e^{-\pi i\varphi})|^{2}$$

$$= \frac{1}{4}|2\cos(\pi\varphi)|^{2}$$

$$= \cos^{2}(\pi\varphi) = \frac{1}{2}(1 + \cos(2\pi\varphi))$$

# Phase kick back due to higher powers of U

For arbitrary k, we obtain

$$|0\rangle - H - \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i 2^k \varphi} |1\rangle)$$

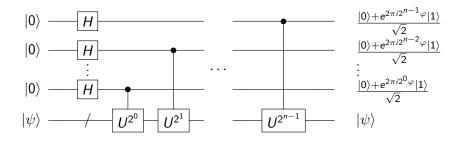
$$|\psi\rangle - H - \psi\rangle$$

$$|\psi\rangle$$

since

$$U^{2^k}|\psi\rangle = e^{2\pi i 2^k \varphi}|\psi\rangle$$

# Phase kick back part of phase estimation



We set

$$|\varphi\rangle:=\frac{|0\rangle+e^{2\pi i 2^{n-1}\varphi}|1\rangle}{\sqrt{2}}\otimes\frac{|0\rangle+e^{2\pi i 2^{n-2}\varphi}|1\rangle}{\sqrt{2}}\otimes\cdots\otimes\frac{|0\rangle+e^{2\pi i 2^0\varphi}|1\rangle}{\sqrt{2}}$$

## Binary fractions

Assume that the eigenphase  $\varphi$  is an exact n-bit binary fraction, i.e.,

$$\varphi = 0.x_1x_2...x_n = \sum_{i=1}^n \frac{x_i}{2^i}$$

For arbitrary  $k \in \{0, \dots, n-1\}$ , we have

$$2^{k} \varphi = x_{1}x_{2} \dots x_{k} \cdot x_{k+1} \dots x_{n}$$

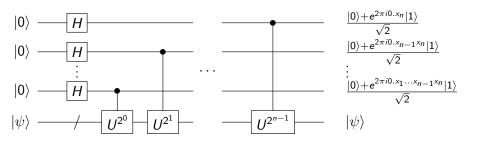
$$e^{2\pi i 2^{k} \varphi} = e^{2\pi i (x_{1}x_{2} \dots x_{k} \cdot x_{k+1} \dots x_{n})}$$

$$= e^{2\pi i (x_{1}x_{2} \dots x_{k} + 0 \cdot x_{k+1} \dots x_{n})}$$

$$= e^{2\pi i (x_{1}x_{2} \dots x_{k})} \cdot e^{2\pi i (0 \cdot x_{k+1} \dots x_{n})}$$

$$= e^{2\pi i (0 \cdot x_{k+1} \dots x_{n})}$$

# Phase kick back part of phase estimation



### Quantum Fourier transform

The quantum Fourier transform F is defined by

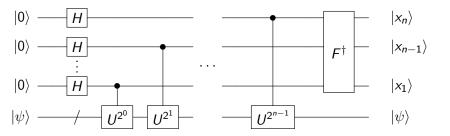
$$F(|x_n\rangle \otimes |x_{n-1}\rangle \otimes \cdots \otimes |x_1\rangle)$$

$$= \frac{|0\rangle + e^{2\pi i 0.x_n} |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + e^{2\pi i 0.x_{n-1}x_n} |1\rangle}{\sqrt{2}} \otimes \cdots \otimes \frac{|0\rangle + e^{2\pi i 0.x_1x_2...x_n} |1\rangle}{\sqrt{2}}$$

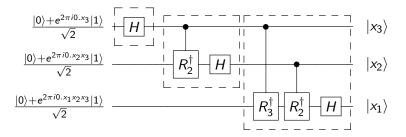
We use inverse quantum Fourier transform  ${\it F}^{\dagger}$  to obtain the bits of the eigenphase

Note: QFT is defined by  $F|x_1\rangle\otimes|x_2\rangle\otimes\cdots\otimes|x_n\rangle=|0.x_1x_2\dots x_n\rangle$  in the literature; we use the above definition for the sake of notational simplicity (otherwise, we would have to include the so-called bit-reversal)

# Quantum circuit for phase estimation



## Inverse quantum Fourier transform for 3 bits



The phase shift  $R_k$  is defined by

$$R_k := \left[ \begin{array}{cc} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{array} \right]$$

# QPE: least significant bit - top qubit

$$\frac{|0\rangle + e^{2\pi i 0.x_3}|1\rangle}{\sqrt{2}} \xrightarrow{\begin{array}{c} - \\ H \end{array}} \frac{|0\rangle + e^{2\pi i 0.x_3}|1\rangle}{\sqrt{2}} = \frac{|0\rangle + (-1)^{x_3}|1\rangle}{\sqrt{2}}$$

$$\xrightarrow{H} |x_3\rangle$$

# QPE: second bit - middle qubit

$$|x_{3}\rangle \qquad |x_{3}\rangle \qquad |x_{3}\rangle \qquad |x_{3}\rangle \qquad |x_{2}\rangle \qquad |x_{2}\rangle \qquad |x_{3}\rangle \qquad |x_{$$

$$|x_{3}\rangle \otimes \frac{|0\rangle + e^{2\pi i 0.x_{2}x_{3}}|1\rangle}{\sqrt{2}}$$

$$\frac{\textit{ctrl R}_{2}^{\dagger}}{\sqrt{2}} \quad |x_{3}\rangle \otimes \frac{|0\rangle + e^{2\pi i 0.x_{2}0}|1\rangle}{\sqrt{2}}$$

$$\frac{\textit{I}\otimes\textit{H}}{\sqrt{2}} \quad |x_{3}\rangle \otimes |x_{2}\rangle$$

# QPE: most significant bit - bottom qubit

$$\begin{array}{c|c} |x_3\rangle & \hline & \hline \\ |x_2\rangle & \hline \\ |x_2\rangle & \hline \\ |\underline{0}\rangle + e^{0.x_1x_2x_3}|1\rangle & \hline \\ |R_3^{\dagger}| & R_2^{\dagger} & H \\ \hline \\ | & & | & | & | \\ \hline \end{array}$$

$$\begin{aligned} |x_3\rangle\otimes|x_2\rangle\otimes\frac{|0\rangle+e^{2\pi i 0.x_1x_2x_3}|1\rangle}{\sqrt{2}}\\ \frac{\mathit{ctrl}\,R_3^\dagger}{} & |x_3\rangle\otimes|x_2\rangle\otimes\frac{|0\rangle+e^{2\pi i 0.x_1x_20}|1\rangle}{\sqrt{2}}\\ \frac{\mathit{ctrl}\,R_2^\dagger}{} & |x_3\rangle\otimes|x_2\rangle\otimes\frac{|0\rangle+e^{2\pi i 0.x_100}|1\rangle}{\sqrt{2}}\\ \frac{\mathit{I}\otimes\mathit{I}\otimes\mathit{H}}{} & |x_3\rangle\otimes|x_2\rangle\otimes|x_1\rangle \end{aligned}$$

## Summary of phase estimation circuit

We use phase kick back due to the controlled  $U^{2^k}$  gate to prepare the state

$$\frac{|0\rangle+e^{2\pi i0.x_{k+1}x_{k+2}...x_n}|1\rangle}{\sqrt{2}}$$

Using the previously determined bits  $x_{k+2}, \dots, x_n$ , we change this state to

$$\frac{|0\rangle+e^{2\pi i0.x_{k+1}0...0}|1\rangle}{\sqrt{2}}=\frac{|0\rangle+(-1)^{x_k}|1\rangle}{\sqrt{2}}$$

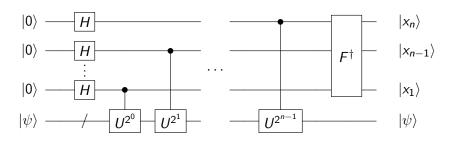
We apply the Hadamard gate to obtain

$$|x_{k+1}\rangle$$

The controlled phase shifts enable us to reduce the problem of determining each bit to distinguishing between  $|+\rangle$  and  $|-\rangle$  (deterministic Hadamard test)

### Special case: exact *n*-bit binary fraction

Assume that  $\varphi$  is an exact *n*-bit binary fraction, i.e.,  $\varphi = 0.x_1 \dots x_{n-1} x_n$ 



 $\Rightarrow$  The measurment of the qubits yields the bits  $x_n, x_{n-1}, \dots, x_1$  deterministically

# General case: arbitrary eigenphases

Let  $\varphi$  be arbitrary

Unless  $\varphi$  is an exact  $\emph{n}\text{-bit}$  fraction, the application of the inverse quantum Fourier transform

$$F^{\dagger}|arphi
angle$$

produces a superposition of *n*-bit strings

### Geometric summation

#### Lemma

We have

$$\sum_{y=0}^{N-1} e^{2\pi i \theta y} = N \text{ for } \theta = 0$$

$$\sum_{y=0}^{N-1} e^{2\pi i \theta y} = \frac{1 - e^{2\pi i N \theta}}{1 - e^{2\pi i \theta}} \text{ for } \theta \in (0,1)$$

Assume that 
$$\theta = \frac{x}{N}$$
 for some  $x \in [0, N-1]$ 

 $\Rightarrow$  We have

$$\sum_{y=0}^{N-1} e^{2\pi i \frac{x}{N}y} = N \, \delta_{x,0}$$

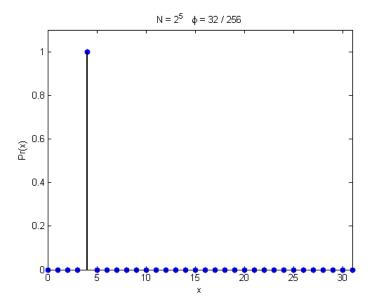
# Probability of obtaining a certain estimate

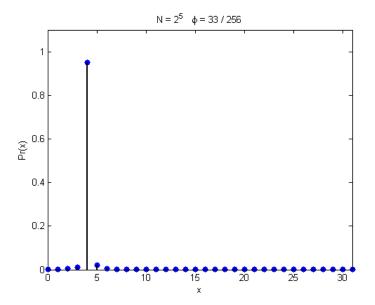
#### Lemma

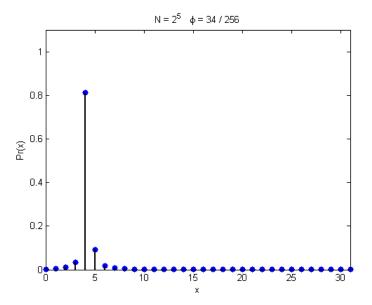
Let  $x = \sum_{k=1}^{n} x_i 2^{n-i}$  and  $\varphi_x := 0.x_1 x_2 \dots x_n = \frac{x}{2^n}$  be the corresponding n-bit fraction

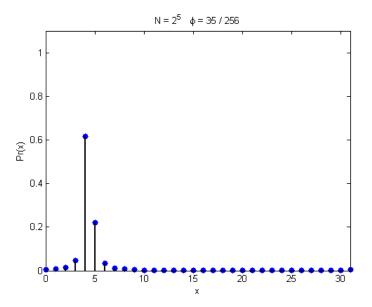
The probability of obtaining the estimate  $\varphi_x$  is

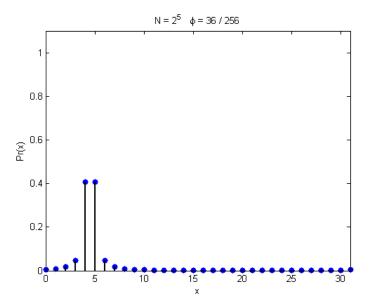
$$Pr(x) = \frac{1}{2^{2n}} \frac{\sin^2 \left(2^n \pi (\varphi - \varphi_x)\right)}{\sin^2 \left(\pi (\varphi - \varphi_x)\right)}$$

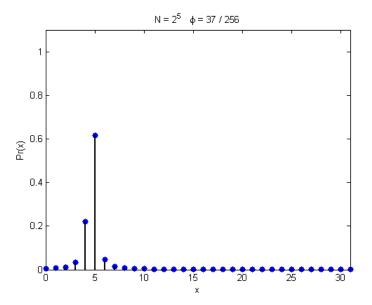


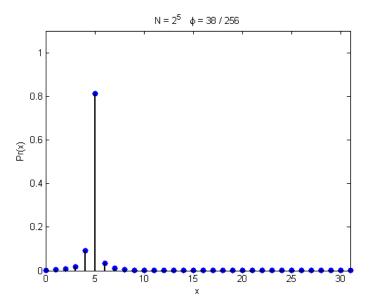


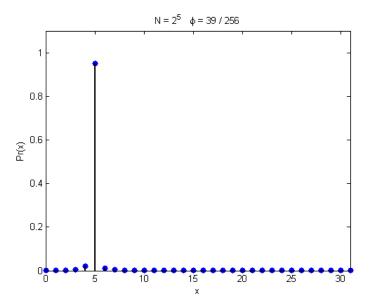


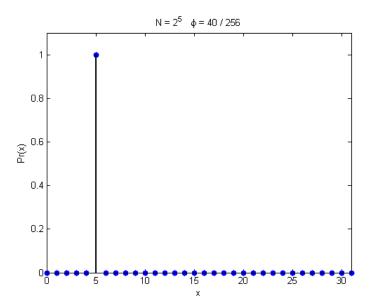












## Probability of obtaining a certain estimate

#### Proof.

The probability of obtaining the estimate  $\varphi_{\mathsf{x}}$  is

$$\begin{aligned} &\operatorname{Pr}(x) \\ &= \ |\langle x|F^\dagger|\varphi\rangle|^2 \\ &= \ |\langle \varphi_x|\varphi\rangle|^2 \\ &= \ \frac{1}{2^{2n}} \Big| \sum_{y=0}^{2^{n-1}} e^{2\pi i (\varphi-\varphi_x)y} \Big|^2 \quad \text{geometric summation} \\ &= \ \frac{1}{2^{2n}} \Big| \frac{1-e^{2\pi i (2^n(\varphi-\varphi_x))}}{1-e^{2\pi i (\varphi-\varphi_x)}} \Big|^2 \quad |1-e^{i2\theta}| = |e^{-i\theta}-e^{i\theta}| = 2|\sin\theta| \\ &= \ \frac{1}{2^{2n}} \frac{\sin^2(2^n \pi(\varphi-\varphi_x))}{\sin^2(\pi(\varphi-\varphi_x))} \end{aligned}$$

## Lower bound on success probability

#### **Theorem**

Let x be such that  $\frac{x}{2^n} \le \varphi < \frac{x+1}{2^n}$ 

The probability of returning one of the two closest n-bit fractions  $\varphi_x$  and  $\varphi_{x+1}$  is at least  $\frac{8}{\pi^2}$ 

# Proof of lower bound on success probability

$$\Pr(\text{success}) := \Pr(x) + \Pr(x+1)$$

$$= \frac{1}{2^{2n}} \left( \left| \sum_{y=0}^{2^{n}-1} e^{2\pi i (\varphi - \varphi_{x})y} \right|^{2} + \left| \sum_{y=0}^{2^{n}-1} e^{2\pi i (\varphi - \varphi_{x})y} \right|^{2} \right)$$

This function attains its minimum at  $\varphi = \frac{1}{2}(\varphi_x + \varphi_{x+1})$  =

$$\text{Pr(success)} \geq \frac{2}{2^{2n}} \left( \left| \sum_{y=0}^{2^{n}-1} e^{2\pi i \frac{y}{2^{n+1}}} \right|^{2} \right)$$

$$\geq \frac{2}{2^{2n}} \frac{4}{4 \sin^{2}(\frac{\pi}{2^{n+1}})}$$

$$\geq \frac{8}{\pi^{2}}$$

The last inequality follows from  $\frac{1}{|\sin\theta|^2} \geq \frac{1}{|\theta|^2}$ 

### Summary of phase estimation

We are given a unitary U and an eigenvector  $|\psi\rangle$  of U with unknown eigenphase  $\varphi$ 

We obtain an estimate  $\hat{\varphi}$  such that

$$\Pr\left(|\hat{\varphi} - \varphi| \le \frac{1}{2^n}\right) \ge \frac{8}{\pi^2}$$

To do this, we need invoke each of the controlled  $U, U^2, \dots, U^{2^{n-1}}$  gates once

We can boost the success probability to  $1-\epsilon$  by repeating the above algorithm  $O(\log(1/\epsilon))$  times and outputting the median of the outcomes

# Phase estimation applied to superpositions of eigenstates

We are given a unitary U with eigenvectors  $|\psi_i\rangle$  and corresponding eigenphases  $\varphi_i$ 

Let

$$|\psi\rangle = \sum_{i} \alpha_{i} |\psi_{i}\rangle$$

What happens if we apply phase estimation to  $|0\rangle^{\otimes n}\otimes |\psi\rangle$ ?

After the *n* phase kick-backs due to  $U^{2^0}$ ,  $U^{2^1}$ , ...  $U^{2^{n-1}}$ , we obtain

$$\sum_{i} \alpha_{i} |\varphi_{i}\rangle \otimes |\psi_{i}\rangle$$

After applying the inverse quantum Fourier transform, we obtain

$$\sum_{i} \alpha_{i} |\tilde{\mathbf{x}}_{i}\rangle \otimes |\psi_{i}\rangle$$

where  $|\tilde{x}_i\rangle$  denotes a superpositions of *n*-bit estimates of  $\varphi_i$ 

# Part VI

**Factoring** 

### The fundamental theorem of arithmetic

#### **Theorem**

Every positive integer larger than 1 can be factored as a product of prime numbers, and this factorization is unique (up to the order of the factors).

$$N=2^{n_2}\times 3^{n_3}\times 5^{n_5}\times 7^{n_7}\times \cdots$$

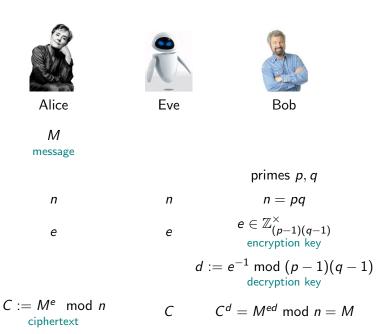
### **Examples**

$$15 = 3 \times 5$$
 
$$239815173914273 = 15485863 \times 15486071$$

 ×  "The problem of distinguishing prime numbers from composite numbers and of resolving the latter into their prime factors is known to be one of the most important and useful in arithmetic. It has engaged the industry and wisdom of ancient and modern geometers to such an extent that it would be superfluous to discuss the problem at length... Further, the dignity of the science itself seems to require that every possible means be explored for the solution of a problem so elegant and so celebrated."

Carl Friedrich Gauss, Disquisitiones Arithmeticæ (1801)

### **RSA**



## Order finding

#### Definition

Given  $a, N \in \mathbb{Z}$  with gcd(a, N) = 1, the *order* of a modulo N is the smallest positive integer r such that  $a^r \equiv 1 \pmod{N}$ .

#### **Problem**

- ▶ Given:  $a, N \in \mathbb{Z}$  with gcd(a, N) = 1
- ► Task: find the order of a modulo N

# Spectrum of a cyclic shift

Let P be a cyclic shift modulo r:  $P|x\rangle = |x+1 \mod r\rangle$ 

For any  $k\in\mathbb{Z}$ , the state  $|u_k\rangle:=\frac{1}{\sqrt{r}}\sum_{x=0}^{r-1}e^{-2\pi\mathrm{i}kx/r}|x\rangle$  is an eigenstate of P.

$$U|u_k\rangle = \frac{1}{\sqrt{r}} \sum_{x=0}^{r-1} e^{-2\pi i k x/r} |x+1 \bmod r\rangle$$

$$= \frac{1}{\sqrt{r}} \sum_{x=0}^{r-1} e^{2\pi i k/r} e^{-2\pi i k(x+1)/r} |x+1 \bmod r\rangle$$

$$= e^{2\pi i k/r} \frac{1}{\sqrt{r}} \sum_{x=1}^{r} e^{-2\pi i k x/r} |x \bmod r\rangle$$

$$= e^{2\pi i k/r} |u_k\rangle$$

### The multiplication-by-a map

Define U by  $U|x\rangle = |ax\rangle$  for  $x \in \mathbb{Z}_N$ .

### Computing U:

$$\begin{array}{ll} |x,0\rangle \mapsto |x,ax\rangle & \text{(reversible multiplication by a)} \\ & \mapsto |ax,x\rangle & \text{(swap)} \\ & \mapsto |ax,0\rangle & \text{(uncompute reversible division by a)} \end{array}$$

High powers of U can be implemented efficiently using repeated squaring

### Spectrum of the multiplication-by-a map

Define U by  $U|x\rangle = |ax\rangle$  for  $x \in \mathbb{Z}_N$ .

Let r be the order of a modulo N. For any  $k \in \mathbb{Z}$ , the state

$$|u_k\rangle := \frac{1}{\sqrt{r}} \sum_{x=0}^{r-1} e^{-2\pi \mathrm{i}kx/r} |a^x \bmod N\rangle$$

is an eigenstate of U with eigenvalue  $e^{2\pi i k/r}$ .

#### Proof.

Same as for the cyclic shift, due to the isomorphism

$$x \bmod r \leftrightarrow a^x \bmod N$$

# Order finding and phase estimation

$$U|u_k\rangle = e^{2\pi i k/r}|u_k\rangle$$

Phase estimation of U on  $|u_k\rangle$  can be used to approximate k/r.

#### Problems:

- We don't know r, so we can't prepare  $|u_k\rangle$ .
- ▶ We only get an approximation of k/r.
- Even if we knew k/r exactly, k and r could have common factors.

# Estimating k/r in superposition

A useful identity:

$$\sum_{k=0}^{r-1} e^{2\pi i k x/r} = \begin{cases} r & \text{if } x = 0\\ 0 & \text{otherwise} \end{cases}$$

Consider

$$\frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} |u_k\rangle = \frac{1}{r} \sum_{k,x=0}^{r-1} e^{-2\pi i kx/r} |a^x \mod N\rangle$$
$$= |a^0 \mod N\rangle = |1\rangle$$

Phase estimation:

$$|0\rangle\otimes|1\rangle=rac{1}{\sqrt{r}}\sum_{k=0}^{r-1}|0\rangle\otimes|u_k\rangle\mapstorac{1}{\sqrt{r}}\sum_{k=0}^{r-1}|\widetilde{k/r}\rangle\otimes|u_k\rangle$$

Measurement gives an approximation of k/r for a random k

### Continued fractions

#### **Problem**

Given samples x of the form  $\lfloor k \frac{2^n}{r} \rfloor$ ,  $\lceil k \frac{2^n}{r} \rceil$   $(k \in \{0, 1, \dots, r-1\})$ , determine r.

Continued fraction expansion:

$$\frac{x}{2^n} = \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \dots}}}$$

Gives an efficiently computable sequence of rational approximations

#### **Theorem**

If  $2^n \ge N^2$ , then k/r is the closest convergent of the CFE to  $x/2^n$  among those with denominator smaller than N.

Since r < N, it suffices to take  $n = 2 \log_2 N$ 

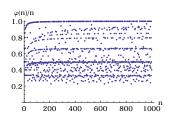
#### Common factors

If gcd(k, r) = 1, then the denominator of k/r is r

#### **Fact**

The probability that  $\gcd(k,r)=1$  for a random  $k \in \{0,1,\ldots,r-1\}$  is

$$\frac{\phi(r)}{r} = \Omega\left(\frac{1}{\log\log r}\right)$$



Thus  $\Omega(\log \log N)$  repetitions suffice to give r with constant probability

Alternatively, find two (or more) denominators and take their least common multiple; then O(1) repetitions suffice

### Factoring → finding a nontrivial factor

Suppose we want to factor the positive integer N.

Since primality can be tested efficiently, it suffices to give a procedure for finding a nontrivial factor of N with constant probability.

```
function factor(N)
if N is prime
    output N
else
    repeat
    x=find_nontrivial_factor(N)
    until success
    factor(x)
    factor(N/x)
end if
```

We can assume N is odd, since it is easy to find the factor 2.

We can also assume that N contains at least two distinct prime powers, since it is easy to check if it is a power of some integer.

### Reduction of factoring to order finding

Factoring N reduces to order finding in  $\mathbb{Z}_N^{\times}$  [Miller 1976].

Choose  $a \in \{2, 3, \dots, N-1\}$  uniformly at random.

If  $gcd(a, N) \neq 1$ , then it is a nontrivial factor of N.

If gcd(a, N) = 1, let r denote the order of a modulo N.

Suppose r is even. Then

$$a^{r} = 1 \mod N$$

$$(a^{r/2})^{2} - 1 = 0 \mod N$$

$$(a^{r/2} - 1)(a^{r/2} + 1) = 0 \mod N$$

so we might hope that  $gcd(a^{r/2}-1, N)$  is a nontrivial factor of N.

### Miller's reduction

#### Question

Given  $(a^{r/2} - 1)(a^{r/2} + 1) = 0 \mod N$ , when does  $gcd(a^{r/2} - 1, N)$  give a nontrivial factor of N?

Note that  $a^{r/2} - 1 \neq 0 \mod N$  (otherwise the order of a would be r/2, or smaller).

So it suffices to ensure that  $a^{r/2} + 1 \neq 0 \mod N$ .

#### Lemma

Suppose  $a \in \mathbb{Z}_N^{\times}$  is chosen uniformly at random, where N is an odd integer with at least two distinct prime factors. Then with probability at least 1/2, the order r of a is even and  $a^{r/2} \neq -1 \mod N$ .

## Proof (part 1 of 2)

Let 
$$N = p_1^{m_1} \times \cdots \times p_k^{m_k}$$
 ( $p_i$  distinct odd primes,  $k \ge 2$ )
$$a = a_i \mod p_i^{m_i}$$

$$r_i = \text{order of } a_i \mod p_i^{m_i}$$

$$2^{c_i} = \text{largest power of 2 that divides } r_i$$

If r is odd or  $a^{r/2} + 1 = 0 \mod N$ , then  $c_1 = \cdots = c_k$ .

Since  $r = \text{lcm}(r_1, \ldots, r_k)$ , r is odd iff  $c_1 = \ldots = c_k = 0$ .

If r is even and  $a^{r/2} = -1 \mod N$ , then  $a^{r/2} = -1 \mod p_i^{m_i}$  for each i, so  $r_i$  does not divide r/2; but notice that  $r_i$  does divide r.

Hence  $r/r_i$  is an odd integer for each i, and every  $r_i$  must contain the same number of powers of 2 as r.

### Proof (part 2 of 2)

$$Pr(c_i = any \ particular \ value) \le 1/2$$

(Then the lemma follows, since in particular  $\Pr(c_1 = c_2) \leq 1/2$ .)

$$a \in \mathbb{Z}_N^{ imes}$$
  $a_i \in \mathbb{Z}_{p_i^{m_i}}^{ imes}$  uniformly at random uniformly at random

Since  $\mathbb{Z}_{p_i^{m_i}}^{\times}$  is cyclic and of even order, exactly half its elements have the maximal value of  $c_i$ , so in particular the probability of any particular  $c_i$  is at most 1/2.

### Shor's algorithm

Input: Integer N

Output: A nontrivial factor of N

- 1. Choose a random  $a \in \{2, 3, \dots, N-1\}$
- 2. Compute gcd(a, N); if it is not 1 then it is a nontrivial factor, and otherwise we continue
- 3. Perform phase estimation with the multiplication-by-a operator U on the state  $|1\rangle$  using  $n=2\log_2 N$  bits of precision
- Compute the continued fraction expansion of the estimated phase, and find the best approximation with denominator less than N; call the result r
- 5. Compute  $gcd(a^{r/2}-1, N)$ . If it is a nontrivial factor of N, we are done; if not, go back to step 1

### Quantum vs. classical factoring algorithms

#### Best known classical algorithm for factoring N

- ▶ Proven running time:  $2^{O((\log N)^{1/2}(\log \log N)^{1/2})}$
- ▶ With plausible heuristic assumptions:  $2^{O((\log N)^{1/3}(\log \log N)^{1/3})}$

#### Shor's quantum algorithm

- ▶ QFT modulo  $2^n$  with  $n = O(\log N)$ : takes  $O(n^2)$  steps
- Modular exponentiation: compute  $a^x$  for  $x < 2^n$ . With repeated squaring, takes  $O(n^3)$  steps
- ▶ Running time of Shor's algorithm:  $O(\log^3 N)$

### Beyond factoring

There are many fast quantum algorithms based on related ideas

- ► Computing discrete logarithms
- Decomposing abelian/solvable groups
- Estimating Gauss sums
- Counting points on algebraic curves
- Computations in number fields (Pell's equation, etc.)
- ► Abelian hidden subgroup problem
- Non-abelian hidden subgroup problem?

### Part VII

# Quantum search

#### Unstructured search

Quantum computers can quadratically outperform classical computers at a very basic computational task, called unstructured search.

There is a set X containing N items, some of which are marked

We are given a Boolean black box  $f:X \to \{0,1\}$  that indicates whether a given item is marked

The problem is to decide if any item is marked, or alternatively, to find a marked item given that one exists

### Applications of unstructured search

Unstructured search can be thought of as a model for solving problems in NP by brute force search

If a problem is in NP, then we can efficiently recognize a solution, so one way to find a solution is to solve unstructured search

Of course, this may not be the best way to find a solution in general, even if the problem is NP-hard

We don't know if NP-hard problems are really "unstructured"

#### Unstructured search

It is obvious that even a randomized classical algorithm needs  $\Omega(N)$  queries to decide if any item is marked

On the other hand, a quantum algorithm can do much better!

#### Phase oracle

We assume that we a unitary operator  $\boldsymbol{U}$  satisfying

$$U|x\rangle = (-1)^{f(x)}|x\rangle = \begin{cases} |x\rangle & x \text{ is not marked} \\ -|x\rangle & x \text{ is marked} \end{cases}$$

### Target state

We consider the case where there is exactly one  $x \in X$  element that is marked; call this element m

Our goal is to prepare the state  $|m\rangle$ 

#### Initial state

We have no information about which item might be marked

 $\Rightarrow$  We take

$$|\psi\rangle := \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle$$

as the initial state

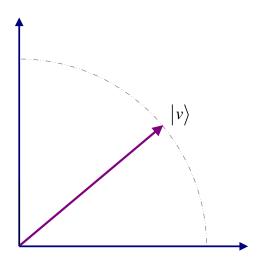
### Rough idea behind Grover search

We start with the initial state  $|\psi\rangle$ 

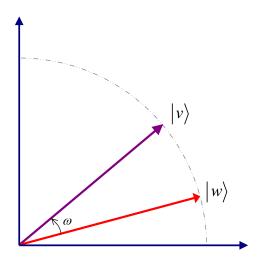
We prepare the target state  $|m\rangle$  by implementing a rotation that moves  $|\psi\rangle$  toward  $|m\rangle$ 

We realize the rotation with the help of two reflections

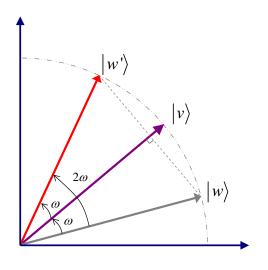
### Visualization of a reflection in $\mathbb{R}^2$



# Visualization of a reflection in $\mathbb{R}^2$



### Visualization of a reflection in $\mathbb{R}^2$



#### Reflections

$$U = I - 2|m\rangle\langle m|$$
 is a reflection about the target state  $|m\rangle$ 

 $V=\mathit{I}-2|\psi\rangle\langle\psi|$  is the reflection around about the initial state  $|\psi\rangle$ :

$$V|\psi\rangle = -|\psi\rangle$$
  
 $V|\psi^{\perp}\rangle = |\psi^{\perp}\rangle$ 

for any state  $|\psi^{\perp}\rangle$  orthogonal to  $|\psi\rangle$ 

#### Structure of Grover

The algorithm is as follows:

- ightharpoonup start in  $|\psi\rangle$ ,
- ightharpoonup apply the Grover iteration G := V U some number of times,
- make a measurement, and hope that the outcome is m

### Invariant subspace

Observe that span $\{|m\rangle,|\psi\rangle\}$  is a U- and V-invariant subspace, and both the inital and target states belong to this subspace

 $\Rightarrow$  It suffices to understand the restriction of VU to this subspace

Consider an orthonormal basis  $\{|m\rangle,|\phi\rangle\}$  for span $\{|m\rangle,|\psi\rangle\}$ 

The Gram-Schmidt process yields

$$|\phi\rangle = \frac{|\psi\rangle - \alpha|m\rangle}{\sqrt{1 - \alpha^2}}$$

where 
$$\alpha := \langle m | \psi \rangle = 1/\sqrt{N}$$

### Invariant subspace

Now in the basis  $\{|m\rangle, |\phi\rangle\}$ , we have

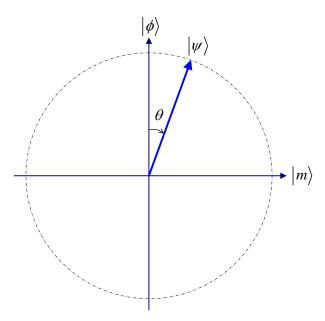
$$\begin{split} |\psi\rangle &= & \sin\theta |m\rangle + \cos\theta |\phi\rangle \text{ where } \sin\theta = \langle m|\psi\rangle = 1/\sqrt{N} \\ U &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\ V &= & I - 2|\psi\rangle \langle \psi| \\ &= & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - 2 \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} \left(\sin\theta & \cos\theta\right) \\ &= & \begin{pmatrix} 1 - 2\sin^2\theta & -2\sin\theta\cos\theta \\ -2\sin\theta\cos\theta & 1 - 2\cos^2\theta \end{pmatrix} \\ &= & - \begin{pmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix} \end{split}$$

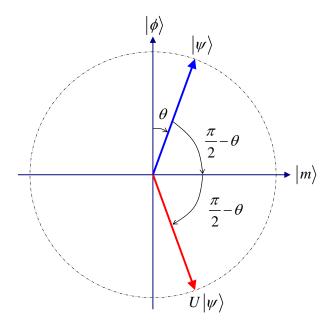
### Grover iteration within the invariant subspace

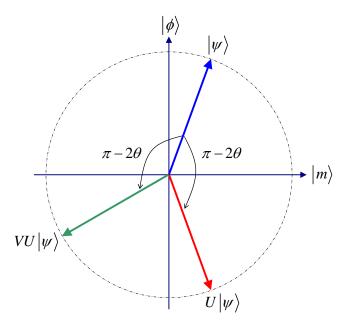
 $\Rightarrow$  We find

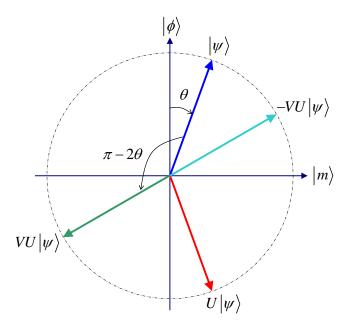
$$V U = -\begin{pmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$= -\begin{pmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{pmatrix}$$

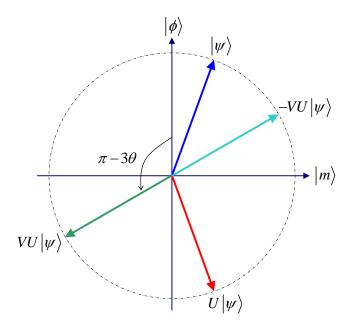
This is a rotation up to a minus sign

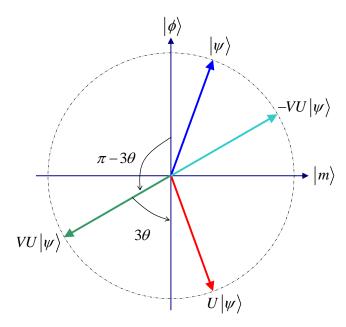


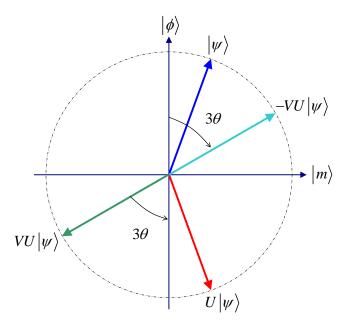


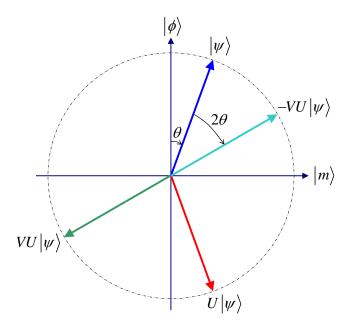












#### Grover search

Geometrically, U is a reflection around the  $|m\rangle$  axis and V is a reflection around the  $|\psi\rangle$  axis, which is almost but not quite orthogonal to the  $|m\rangle$  axis

The product of these two reflections is a clockwise rotation by an angle  $2\theta$ , up to an overall minus sign

From this geometric picture, or by explicit calculation using trig identities, it is easy to verify that

$$(VU)^k = (-1)^k \begin{pmatrix} \cos 2k\theta & \sin 2k\theta \\ -\sin 2k\theta & \cos 2k\theta \end{pmatrix}$$

#### Grover search

Recall that our initial state is  $|\psi\rangle = \sin\theta |m\rangle + \cos\theta |\phi\rangle$ 

How large should k be before  $(VU)^k|\psi\rangle$  is close to  $|m\rangle$ ?

We start an angle  $\theta$  from the  $|\phi\rangle$  axis and rotate toward  $|m\rangle$  by an angle  $2\theta$  per iteration

 $\Rightarrow$  To rotate by  $\pi/2$ , we need

$$heta + 2k heta = \pi/2$$
 
$$k \approx \frac{\pi}{4}\theta^{-1} \approx \frac{\pi}{4}\sqrt{N}$$

#### Grover search

It is easy to calculate that

$$|\langle m|(VU)^k|\psi\rangle|^2 = \sin^2((2k+1)\theta)$$

This is the probability that, after k steps of the algorithm, a measurement reveals the marked state

We are solving a completely unstructured search problem with N possible solutions, yet we can find a unique solution in only  $O(\sqrt{N})$  queries!

While this is only a polynomial separation, it is very generic, and it is surprising that we can obtain a speedup for a search in which we have so little information to go on

#### Grover search

It can also be shown that this quantum algorithm is optimal

Any quantum algorithm needs at least  $\Omega(\sqrt{N})$  queries to find a marked item (or even to decide if some item is marked)

### Multiple solutions

Assume that there are t marked items

 $\Rightarrow$  There is a two-dimensional invariant subspace spanned by  $\mathrm{span}\{|\mu\rangle,|\psi\rangle\}$  where

$$|\mu\rangle = \frac{1}{\sqrt{t}} \sum_{x \, \text{marked}} |x\rangle$$

is the uniform superposition of all solutions

The Gram-Schmidt process yields the ONB  $\{|\mu\rangle, |\phi\rangle\}$  where

$$|\phi\rangle = \frac{1}{\sqrt{N-t}} \sum_{\text{x unmarked}} |x\rangle$$

is the uniform superposition of all non-solutions

### Invariant subspace

Now in the basis  $\{|\mu\rangle, |\phi\rangle\}$ , we have

$$\begin{split} |\psi\rangle &=& \sin\theta |\mu\rangle + \cos\theta |\phi\rangle \text{ where } \sin\theta = \langle\mu|\psi\rangle = \sqrt{\frac{t}{N}} \\ VU &=& -\begin{pmatrix} \cos2\theta & \sin2\theta \\ -\sin2\theta & \cos2\theta \end{pmatrix} \end{split}$$

# Overshooting

The success probability is given by

$$\sin((2k+1)\theta)$$
 where  $\sin\theta=\sqrt{\frac{t}{N}}$ 

 $\Rightarrow$  We need to apply VU

$$k \approx \frac{\pi}{4} \sqrt{\frac{N}{t}}$$

times

Due to the oscillatory behaviour of the success probability it is important not to overshoot, i.e., to choose a number of iterations that it too large, so that the probability starts decreasing

### Quantum counting

The eigenvalues of

$$-VU = \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{pmatrix}$$

are  $e^{i2\theta}$  and  $e^{-i2\theta}$ 

The initial state  $|\psi\rangle$  is a superposition of the two eigenvectors corresponding to the above two eigenvalues

 $\Rightarrow$  Using phase estimation, we can obtain an estimate  $ilde{ heta}$  such that

$$|\theta - \tilde{\theta}| \le \epsilon$$

by invoking the controlled version of -VU

$$O(1/\epsilon)$$
 times

# Quantum counting

Using the estimate  $\tilde{\theta},$  we obtain an estimate  $\tilde{t}$  satifying

$$|t - \tilde{t}| \le (2\sqrt{tN} + \epsilon)\epsilon$$

### Quantum counting

We use the following two inequalities:

$$\begin{split} |\sin\theta + \sin\tilde{\theta}| & \leq 2\sin\theta + |\theta - \tilde{\theta}| \leq 2\sqrt{\frac{t}{N}} + \epsilon \\ |\sin\theta - \sin\tilde{\theta}| & \leq |\theta - \tilde{\theta}| \leq \epsilon \end{split}$$

We have

$$\begin{split} \left| \frac{t}{N} - \frac{\tilde{t}}{N} \right| &= |\sin^2 \theta - \sin^2 \tilde{\theta}| \\ &= |\sin \theta + \sin \tilde{\theta}| |\sin \theta - \sin \tilde{\theta}| \\ &\leq \left( 2\sqrt{\frac{t}{N}} + \epsilon \right) \epsilon \end{split}$$

#### Amplitude amplification

Assume that there is a classical (randomized) algorithm that produces a solution to some problem with probability p

Assume that we can recognized if the output produced by the algorithm is a valid solution or not

⇒ We repeat the algorithm until we obtain a solution

The expected number of times we have to repeat is O(1/p) (geometric random variable)

Quantum amplitude amplification makes it possible to reduce the complexity to  $O(1/\sqrt{p})$ 

# Part VIII

Quantum complexity classes

#### Complexity Zoo

Complexity Zoo https://complexityzoo.uwaterloo.ca/Complexity\_Zoo https://complexityzoo.uwaterloo.ca/Zoo\_Intro

# P – Polynomial

https://complexityzoo.uwaterloo.ca/Petting\_Zoo#P

# BPP – Bounded Probabilistic Polynomial

https://complexityzoo.uwaterloo.ca/Petting\_Zoo#BPP

# BQP - Bounded Quantum Polynomial

```
https://complexityzoo.uwaterloo.ca/Complexity_Zoo: B#bqp
```

#### $BQP \subseteq PSPACE$

J. Preskill
Chapter 6 Quantum computation
http://www.theory.caltech.edu/people/preskill/ph229/
notes/chap6.pdf
page 26

# NP – Nondeterministic Polynomial

```
\verb|https://complexityzoo.uwaterloo.ca/Complexity_Zoo: N#np| \\
```

# NP-complete

```
\verb|https://complexityzoo.uwaterloo.ca/Complexity_Zoo: N#npc| \\
```

#### MA - Merlin Arthur

https://complexityzoo.uwaterloo.ca/Petting\_Zoo#MA

# QMA - Quantum Merlin Arthur

# Local Hamiltonian problem is QMA-complete

D. Aharonov and T. Naveh
Quantum NP - a survey
https://arxiv.org/pdf/quant-ph/0210077.pdf