

Unit 04: Grinding Gates in Quantum Computers

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(Dated: August 28, 2026)

In this unit, we discuss the standard circuit-based quantum computation (and introduce Qiskit developed by IBM).

Learning outcomes: (1) You'll be able to know elementary single-qubit and two-qubit quantum gates. (2) You'll be able to understand what quantum computation is and the specific quantum algorithm on searching. (3) You'll be able to get started in IBM Qiskit and run simple Jupyter notebooks of quantum circuits. [Note that the introduction of using IBM Qiskit will be moved to another course PHY605 Quantum Programming.]

I. INTRODUCTION

We will now give an overview of quantum computation in terms of the standard circuit model. You have seen all the necessary ingredients before, and these are: (1) Initialization, (2) Gate operations and (3) Measurement/Readout. The schematic circuit is shown in Fig. 1.

In the initialization, we usually assume that all qubits are initialized to $|0\rangle$, unless stated otherwise. The specific layout of gate operations does not need to resemble that shown in the figure and it may depend on how an n -qubit unitary U is decomposed into a sequence of one-qubit and two-qubit gates. This second ingredient is the crux of quantum computation. To read out results, we need to perform measurement and it is usually assumed that each qubit is measured in the 0/1 or equivalently Z basis. If we need to measure in $+/-$ basis, we can apply a Hadamard gate H right before the 0/1 measurement.

Universal gate set. In classical computation, AND and NOT gates or just NAND gates are sufficient to build any Boolean functions. They are regarded as universal gate sets. In quantum computation, we also have the similar notion of universality. Given any unitary U acting on n -qubit, i.e., a unitary matrix of dimension $2^n \times 2^n$, it can be decomposed into a sequence of single-qubit and two-qubit gates. This is described in detail in Chapter 4 section 5 of Nielsen and Chuang. Essentially, the unitary U is decomposed into a sequence of the so-called two-level unitaries, each of which is a nontrivial action on a two-dimensional subspace, i.e., a multi-controlled-single-qubit unitary gates, i.e., the number of them is at most $2^{n-1}(2^n - 1)$. Then as we shall see below in some examples of gate identity, each multi-controlled gates can in turn be decomposed into single-qubit gates and CNOT gates. This means that the set of arbitrary single-qubit gates and the CNOT gate constitutes the corresponding universal set of gates in quantum computing. We note that the decomposition of U in the set is exact.

Exercise. What is the upper bound on the number of CNOT gates needed to implement an arbitrary U ? Note that for a k -qubit controlled single-qubit gate (in total a $(k + 1)$ -qubit gate), one can use $2k - 2$ Toffoli gates (see below) and single-qubit controlled single qubit gate (in total a 2-qubit gate).

You may have also heard people say that H , T and CNOT constitute a universal gate set, where we have seen H and CNOT, and T gate is

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix},$$

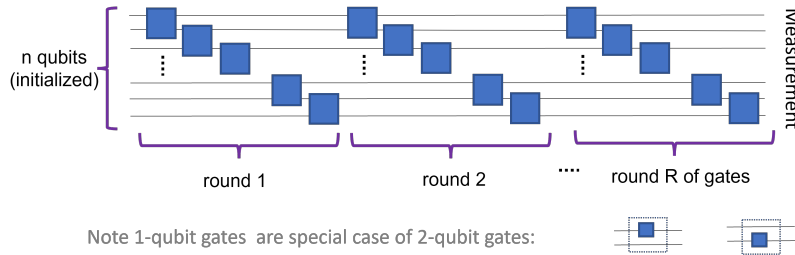


FIG. 1. Illustration of quantum computation in terms of the standard circuit model. We also note that one-qubit gates are a special case of two-qubit gates.

which can be regarded as a $\pi/4$ rotation about the z-axis: $T = e^{i\pi/8}e^{-i(\pi/4)(Z/2)}$. However, there are two fine-grained details. First, these three gates together *cannot* exactly constitute an arbitrary unitary U , but *can approximate* it as close as possible. This is the approximate universality. There are two other examples of such approximate universal gate sets.

- Example 2:

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \text{Controlled} - \text{HZ} = \text{---} \bullet \text{---} \begin{array}{c} \boxed{\text{HZ}} \\ \text{---} \end{array}, \quad \text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \text{---} \times \text{---}$$

- Example 3:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{Toffoli} = C^2 - X (\text{Control-Control-NOT}) = \text{---} \bullet \text{---} \oplus \text{---}$$

The last two examples give other universal gates but achieve arbitrary gates in an approximate way. They also illustrate that universal quantum computation can be done with real-valued gates only. We note that the number i is essential in quantum mechanics [1, 2], though.

The exact universal set of gates includes all the one-qubit gates $u3(\theta, \phi, \lambda)$ and the CNOT gate (or equivalently C-Z gate for the latter); the specific form of $u3$ is

$$u3(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda} \sin(\theta/2) \\ e^{i\phi} \sin(\theta/2) & e^{i\lambda+i\phi} \cos(\theta/2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix} = e^{i(\phi+\lambda)/2} e^{-i\phi Z/2} e^{-i\theta Y/2} e^{-i\lambda Z/2}, \quad (1)$$

which is a rotation using Euler angles: first around z by λ , then around y by θ , followed by rotation around z by ϕ .

Further comments on universality. It is recommended to read through Chapter 4.5 of Nielsen and Chuang on universal quantum gates. They illustrate that “two-level” unitary gates are universal, which basically shows that any $d \times d$ unitary matrix can be decomposed to a product at most $d(d-1)/2$ unitary gates, each of which is almost identity, except at a 2×2 block inside the matrix. This was done by a procedure similar to Gauss elimination, except that we have to use unitary matrices. Afterwards, one needs to show that any such two-level unitary gate can be decomposed as multi-qubit controlled NOT gates and multi-qubit controlled unitary gates (with the same 2×2 block). This establishes the exact universality of using CNOT gates and arbitrary one-qubit gates.

For a discrete set of universal gates, one needs to equip with the notion of approximation. For example, with H and T gates, one can generate a rotation by an angle that is an irrational multiple of 2π . This allows to approximate any single-qubit rotation gate as close as possible by using a longer sequence of H and T gates. The essential equation is

$$e^{-i\frac{\pi}{8}Z} e^{-i\frac{\pi}{8}X} = \cos^2 \frac{\pi}{8} I - i \sin \frac{\pi}{8} \left[\cos \frac{\pi}{8} (X + Z) + \sin \frac{\pi}{8} Y \right],$$

i.e., a rotation about an axis $\vec{n} = (\cos \frac{\pi}{8}, \sin \frac{\pi}{8}, \cos \frac{\pi}{8})$ (un-normalized) by an angle θ with $\cos(\theta/2) = \cos^2 \frac{\pi}{8}$. We thus need an efficient way to approximate a unitary using discrete gates. If it costs an exponential number of gates to reach the accuracy being ϵ , then the decomposition will not be useful. Naively, if we want to approximate an m -gate circuit to accuracy ϵ , the number of gates from a fixed set required scales as $\Theta(m^2/\epsilon)$. In general, approximating arbitrary unitary gates is hard. This can be understood by a counting argument, by asking the alternative question that how many gates it takes to create an arbitrary n -qubit state. This can be done by using the ϵ -net picture; see Nielsen and Chuang 4.5.4. Fortunately, there is a much better convergence according to the Solovay-Kitaev theorem, which uses $O(\log^c(1/\epsilon))$ gates from the set to achieve the same accuracy ϵ . The lower the c is the more efficient one can approximate any unitary gate. It was believed that c can be 1 for any universal gate set, but it was only proven for algebraic gate sets by Bourgain and Gamburd [3], which was an existence proof [4]. For using Clifford+ T gates, Ross and Selinger showed the optimal approximation of z-rotations achieves $c = 1$, and they provided an probabilistic algorithm [5]. In a homework problem in Appendix 3 of Nielsen and Chuang, $c = 2 + \delta$ for an arbitrary universal gate set is claimed but the argument outlined there looks incorrect. The book by Kitaev, Shen, and Valyi properly established $c = 3 + \delta$ for an arbitrary gate set and supplied with an efficient algorithm [6]. This important result was recently improved by Kuperberg to $c > 1.44042$ [7].

II. GATE IDENTITIES AND MULTIQUBIT GATE DECOMPOSITION

Gate identities are useful in simplifying circuits and in proving circuit equivalence. Sometimes, they help to understand certain symmetry and properties of the state generated, e.g., the cluster states that we will see in a later unit on measurement-based quantum computation.

Gate identities. The first one we have seen earlier is the transformation between x and z bases via the Hadamard gate,

$$-\boxed{X}-\boxed{H}- = -\boxed{H}-\boxed{Z}-$$

How do we transform between x and y bases? It is done via the phase gate,

$$S \equiv \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad SX S^\dagger = Y.$$

Given CNOT's importance as a two-qubit gate, we examine how it commutes with X and Z gates.

$$\begin{array}{ccc} \begin{array}{c} \text{---} \boxed{Z} \text{---} \\ \bullet \\ \text{---} \oplus \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{Z} \text{---} \end{array} \end{array} \quad \begin{array}{ccc} \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{Z} \text{---} \oplus \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{Z} \text{---} \end{array} \end{array}$$

$$\begin{array}{ccc} \begin{array}{c} \text{---} \boxed{X} \text{---} \\ \bullet \\ \text{---} \oplus \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{X} \text{---} \end{array} \end{array} \quad \begin{array}{ccc} \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{X} \text{---} \oplus \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{X} \text{---} \end{array} \end{array}$$

We can also conjugate controlled gates by a single-qubit unitary at the target,

$$\begin{array}{ccc} \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{V} \text{---} \boxed{U} \text{---} \boxed{V^\dagger} \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \boxed{V^\dagger U V} \text{---} \end{array} \end{array} \quad \begin{array}{ccc} \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{H} \text{---} \boxed{X} \text{---} \boxed{H} \text{---} \end{array} & = & \begin{array}{c} \bullet \\ \text{---} \boxed{Z} \text{---} \end{array} =: \begin{array}{c} \bullet \\ \bullet \end{array}$$

To build a swap gate between two qubits requires three CNOTs,

$$\begin{array}{c} \times \\ \times \end{array} = \begin{array}{c} \bullet \oplus \bullet \\ \oplus \bullet \oplus \end{array}$$

A controlled phase gate is similar to the phase kickback,

$$\begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{e^{i\alpha} I} \text{---} \end{array} = \begin{array}{c} \text{---} \boxed{u1(\alpha)} \text{---} \end{array}, \quad u1(\alpha) \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix}$$

Multiqubit gates from the standard set. There are a few useful identities for us to construct multiqubit gates. But first we look at the two-qubit gate,

$$\begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{U} \text{---} \end{array} = \begin{array}{c} \bullet \\ \text{---} \oplus \text{---} \bullet \text{---} \boxed{u1(\alpha)} \text{---} \\ \text{---} \boxed{C} \text{---} \oplus \text{---} \boxed{B} \text{---} \oplus \text{---} \boxed{A} \text{---} \end{array} \quad (2)$$

This is based on the single-qubit U being decomposed to $U = e^{i\alpha} A X B X C$, with $ABC = I$. The next is a three-qubit controlled gate,

$$\begin{array}{c} \bullet \\ \bullet \\ \text{---} \oplus \text{---} \\ \text{---} \boxed{U} \text{---} \end{array} = \begin{array}{c} \bullet \bullet \bullet \\ \text{---} \oplus \text{---} \oplus \text{---} \oplus \text{---} \\ \text{---} \boxed{V} \text{---} \oplus \text{---} \boxed{V^\dagger} \text{---} \oplus \text{---} \boxed{V} \text{---} \end{array} \quad (3)$$

where $V^2 = U$. For Toffoli gate: $U=X$, so can choose the following V and then the controlled- V ,

$$V = \frac{1-i}{2}(I + iX) \Rightarrow V^2 = X.$$

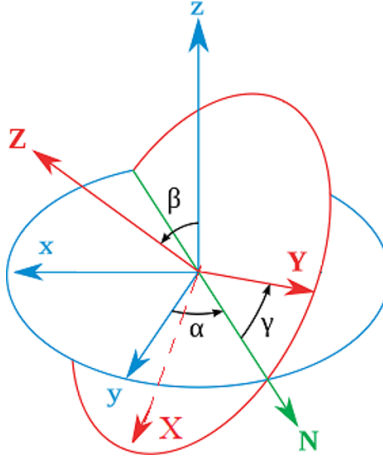
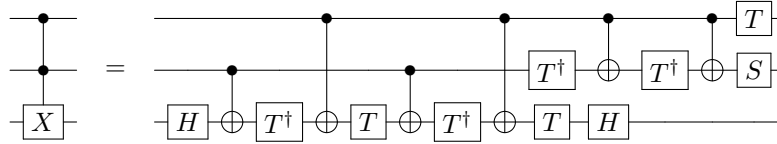


FIG. 2. Illustration of Euler rotations: how two sets of coordinate frames can be rotated to each other. The two x-y and X-Y planes intersect along the N axis. It is thus clear that the two axes z and Z are orthogonal to N . To align the two frames, one rotate y axis around z axis (by an angle α) so that y axis aligns with the N axis. Then one rotate z axis about N to align with the Z axis by an angle β . Finally, one rotates the y axis (now with N) around the Z axis by an angle γ to align with the Y axis. The x and X axes will then be aligned automatically.

This requires 8 CNOT gates. But there is a decomposition with 6 CNOT gates



This is left as an exercise. We note that there is a proof that there must be at least 5 two-qubit gates for the Toffoli gate [8], and the use of Eq. (3) will achieve this.

In the book by Nielsen and Chuang, there is some discussion on n -qubit controlled unitary, but we will not cover it here. For example, in their Fig. 4.10, you can construct an n -qubit controlled U gate by using $n - 1$ ancillary qubits, $2(n - 1)$ Toffoli gates and one $c-U$ gate. Additionally, we note that there is an interesting construction of a single-qubit controlled version of unitary U (or any quantum operation O), which can be unknown, using ancillas or an extended Hilbert space [9].

Euler rotation. According to the steps in Fig. 2, the overall rotation is described by

$$U(\alpha, \beta, \gamma) = R_Z(\gamma)R_N(\beta)R_z(\alpha).$$

We will need the two identities

$$R_Z(\gamma) = R_N(\beta)R_z(\gamma)R_N(\beta)^{-1}, \quad R_N(\beta) = R_z(\alpha)R_y(\beta)R_z(\alpha)^{-1},$$

which simply come from the fact that a rotation by one axis can be done by first rotating the vector to a second axis, then rotating around this axis by the desired angle, and finally rotating from the second axis back to the first. We then rewrite the above U with mixed axes to one with the fixed axes,

$$U(\alpha, \beta, \gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma),$$

whose proof is left as an exercise.

We also include an arbitrary overall phase in the unitary group and for one qubit we have

$$e^{i\delta}U(\alpha, \beta, \gamma) = e^{i\delta}R_z(\alpha)R_y(\beta)R_z(\gamma).$$

The IBM's $u3$ gate (see above Eq. 1) is related to this via $\delta = \frac{\alpha+\gamma}{2}$, $\beta = \theta$, $\alpha = \phi$, $\gamma = \lambda$.

Relating back to the decomposition of control- U in Eq. (2), for the above Euler decomposition, one can verify that $A = R_z(\alpha)R_y(\beta/2)$, $B = R_y(-\beta/2)R_z(-(\gamma+\alpha)/2)$ and $C = R_z((\gamma-\alpha)/2)$, which is left as an exercise (noting that $R_{y,z}(\theta)X = XR_{y,z}(-\theta)$).

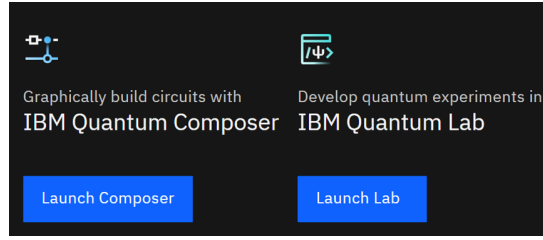


FIG. 3. Illustration of part of the view in a Qiskit account. You can access IBM Quantum at <https://quantum-computing.ibm.com/>. If you are new to IBM Quantum, you can create an IBMid to access it. Two key components to write and run codes are: (1) IBM Quantum Composer and (2) IBM Quantum Lab. [Update: IBM cancelled their Quantum Lab service on May 2024. In order to run Qiskit codes, you will need to install Qiskit on your machine or use other online platforms, such as Google's Colab.]

III. IBM QISKIT: AN INTRODUCTION

A. Register for an account

Please go to <https://quantum-computing.ibm.com/> to register an account. After logging in to your account, you will see (1) IBM Quantum Composer and (2) IBM Quantum Lab among other things, as illustrated in Fig. 3.

B. Qiskit gate set

Here, we list a gates that are available on IBM Qiskit [10]. (We note that some conventions have changed, e.g. gates `u3` and `u2`, will be lumped into a single `u` gate and `u1` gate is renamed as 'p' gate. This also affect their controlled versions.)

u gates.

- `u3(angle1,angle2,angle3):`

$$u3(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda} \sin(\theta/2) \\ e^{i\phi} \sin(\theta/2) & e^{i\lambda+i\phi} \cos(\theta/2) \end{pmatrix}$$

- `u2(angle1,angle2):`

$$u2(\phi, \lambda) = u3(\pi/2, \phi, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i(\phi+\lambda)} \end{pmatrix}$$

- `u1(angle1):`

$$u1(\lambda) = u3(0, 0, \lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$

Identity gate: `iden = u0(angle)`,

$$u0(\delta) = u3(0, 0, 0)$$

Hadamard gate: `h`.

Phase gate and its inverse: `s` and `sdg`.

T gate and its inverse: `t` and `tdg`.

Rotations about X,Y,Z axes: `rx(angle,qubit)`, `ry(angle,qubit)` and `rz(angle,qubit)`.

There are multiple qubit gates.

Controlled-NOT gate: `cx(control,target)`.

Controlled-Y and -Z gates: `cy(control,target)` and `cz(control,target)`.

Controlled-Hadamard gate: `ch(control,target)`.

Controlled-Rotation gates: `crx(angle,control,target)`, `cry(angle,control,target)` and `crz(angle,control,target)`.

Controlled-U1 gate: `cu1(angle,control,target)`.

Controlled-U3 gate: `cu3(angle1,angle2,angle3,control,target)`.

Swap gate: `swap(qubit1,qubit2)`.

Toffoli gate: `ccx(control1,control2,target)`.

Controlled swap gate (Fredkin gate): `cswap(control,qubit2,qubit3)`.

The following are not unitary operations. **Measurement:** `measure(qubit, classical bit)`.

Reset qubit to 0: `reset(qubit)`.

Conditional operation (on classical outcome):

```
qc.measure(q, c)
qc.x(q[0]).c_if(c, 0) # apply X to q[0] if c is 0
```

C. Measurement

In IBM, Google or Rigetti, the measurement is done in 0/1 basis, e.g.

```
>>> qc.measure(q, c)
```

In order to measure in arbitrary basis defined by $|\xi(0)\rangle$ and $|\xi(1)\rangle$:

$$|\xi_+\rangle = U_\xi|0\rangle, \quad |\xi_-\rangle = U_\xi|1\rangle,$$

we first apply inverse of U (i.e. $U^\dagger$) before measuring in 0/1 basis,

$$|\psi\rangle \xrightarrow{|\xi_\pm\rangle} = |\psi\rangle \xrightarrow{U^\dagger} \xrightarrow{0/1}$$

Note if one cares about the exact post-measurement state being in the $|\xi\rangle$ basis, one should apply U after the measurement to undo the basis change $U^\dagger$ done earlier.

How to measure a single-qubit operator O (unitary and Hermitian, thus $O^2 = I$) and leave the output in the eigenstate? It can be done with the following circuit (a kind of Hadamard test),



Principle of deferred measurement. In principle, measurement can be moved to the end of the circuit; if measurement results are used to classically control some operation, it can be replaced by a corresponding controlled operation.

IV. CLIFFORD GATES AND GOTTESMAN-KNILL NO-GO THEOREM

Clifford gates U_C 's are those that transform a Pauli product σ to another Pauli product operator σ' (up to $\pm 1, \pm i$):

$$U_C \sigma U_C^\dagger = \sigma'.$$

For one qubit, we have seen example gates that do this: $\{H, S\}$. Of course, Pauli gates X, Y, Z are also other examples, albeit trivial, as they commute or any commute with each other. In fact, the Pauli gates can be generated by $\{H, S\}$, e.g. $Z = S^2$, and $X = HS^2H$. It turns one-qubit Clifford group is generated by H and S , i.e. $\mathcal{C}_1 = \langle\langle H, S \rangle\rangle$. Moreover, for multiple qubit Clifford group, we need additionally CNOT gates.

Given that the transformation by the Clifford group can be identified by how Pauli products are transformed, quantum computation using only these gates (and simple measurements) can be efficiently simulated.

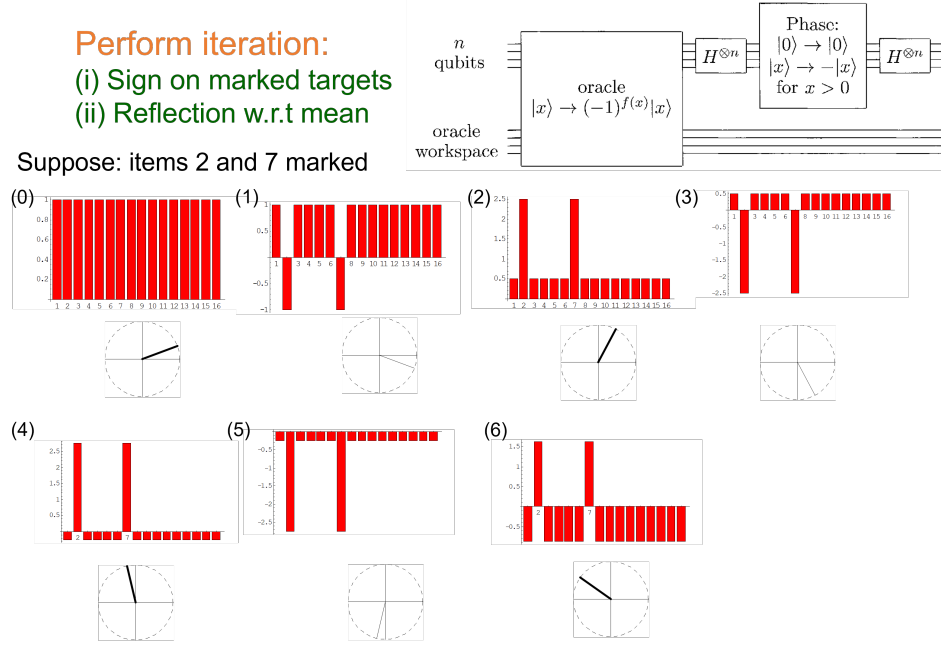


FIG. 4. Illustration of Grover's algorithm on 16 objects with 2 marked items.

We note that how to efficiently represent elements in the Clifford group by quantum circuits is still an important issue; see, e.g., the recent work by Bravyi and Maslov [11], in which they consider the Hadamard-free implementation. Moreover, in a later lecture on MBQC, Clifford operation can be done by measurement in one single step.

The following is a no-go result on the quantum computational power using certain elements.

Theorem 10.7 [of Nielsen and Chuang]: (Gottesman–Knill theorem) Suppose a quantum computation is performed which involves only the following elements: state preparations in the computational basis, Hadamard gates, phase gates, controlled-NOT gates, Pauli gates, and measurements of observables in the Pauli group (which includes measurement in the computational basis as a special case), together with the possibility of classical control conditioned on the outcome of such measurements. Such a computation may be efficiently simulated on a classical computer.

For the proof, please refer to N&C. We remark that the Pauli group (generated by Pauli products) is referred to as the first hierarchy $\mathcal{C}^{(1)}$ in the Clifford hierarchy, while the Clifford group is in the second hierarchy $\mathcal{C}^{(2)}$. The hierarchy is defined iteratively, those in hierarchy $\mathcal{C}^{(k+1)}$ transform any Pauli product to some element in $\mathcal{C}^{(k)}$. Examples elements in the third hierarchy includes the T gate and the Toffoli gate CCX or its cousin CCZ gate. They are needed for universal quantum computation that cannot be efficiently simulated by classical computers. The structure of higher Clifford hierarchy is still an active research: for example, diagonal elements were understood well [12] in prime dimensions, and elements in $\mathcal{C}^3$ can be expressed in terms of Clifford-Permutation-Diagonal-Clifford, but largely unknown for higher hierarchies; see e.g., [13] for the study on permutations.

V. GROVER'S SEARCH ALGORITHM

We continue the rest of the unit by discussing Grover's search algorithm and its generalization. Let us refer to Fig. 4 for an illustration of Grover's search algorithm [14–16]. The algorithm involves these following steps ,

- (i) Flip the sign on marked targets (equivalent to reflection w.r.t. the unmarked “plane”):

$$\hat{O}_f = \sum_x (-1)^{f(x)} |x\rangle\langle x| = I - 2 \sum_{x \in \text{marked}} |x\rangle\langle x|.$$

- (ii) Reflection w.r.t. to the mean:

$$U_s = 2|s\rangle\langle s| - I = H^{\otimes n}(2|0\dots 0\rangle\langle 0\dots 0| - I)H^{\otimes n},$$

where

$$|s\rangle = |++\cdots+\rangle = \frac{1}{\sqrt{N=2^n}} \sum_{x=0}^{2^n-1} |x\rangle.$$

Under this,

$$|\alpha\rangle \equiv \sum_k \alpha_k |k\rangle \longrightarrow 2|s\rangle\langle s|\alpha\rangle - |\alpha\rangle,$$

in terms of the components,

$$\alpha_k \longrightarrow 2\frac{1}{N} \sum_j \alpha_j - \alpha_k = 2\langle\alpha\rangle - \alpha_k.$$

These two steps are reflections. One Grover iteration is a combination of the two and is thus a unitary operation that is equivalent to a rotation:

$$\hat{G} \equiv U_s \hat{O}_f,$$

with the angle θ satisfying

$$\sin \theta = 2 \frac{\sqrt{N_{\text{mark}}(N - N_{\text{mark}})}}{N}.$$

This is illustrated in Fig. 5. The goal is to reach $\theta = \pi/2$ as close as possible, and the number of iterations to reach the angle $\pi/2$ is

$$N_{\text{iter}} \theta + \frac{\theta}{2} \approx \frac{\pi}{2}, \quad N_{\text{iter}} \approx \frac{\pi}{2\theta} - \frac{1}{2} \approx \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{N_{\text{mark}}}} \right\rceil.$$

When there is just one marked item $N_{\text{mark}} = 1$,

$$N_{\text{iter}} \approx \left\lceil \frac{\pi\sqrt{N}}{4} \right\rceil,$$

meaning that there is a speedup compared to classical search that needs to examine on average $N/2$ items.

Note that for $N = 4$ with only one marked item: $\theta = \pi/3$, one iteration reaches the target with probability 1. In fact, it is possible to reach an marked item with uncertainty for arbitrary N by, e.g., modifying the action of the oracle (e.g., to have a phase $\phi \neq \pi$ but dependent on N); see, e.g., Refs. [17–19].

When the number of marked items is unknown. How do we know when to stop? This requires the knowledge of the angle θ , which can be estimated using the quantum phase estimation algorithm, which we will discuss in a later lecture. Essentially, the Grover operator $\hat{G}$ has two eigenvalues $e^{\pm i\theta}$. [This is left as an exercise.] If one can imprint the phase to a quantum register then we can read it out using the so-called quantum Fourier transform, which is part of the quantum phase estimation algorithm to be discussed later. Alternatively, one can employ some randomness in the algorithm that can achieve the same scaling; see Theorem 3 of Ref. [17].

VI. GENERALIZATION: AMPLITUDE AMPLIFICATION

Amplitude amplification [17] generalizes the Grover's algorithm and we do not need to create an equal superposition of all objects. Let us recall the case for Grover.

$$\hat{G} \equiv U_s \hat{O}_f = H^{\otimes n} U_{|0\rangle^\perp} H^{\otimes n} \hat{O}_f,$$

where

$$\hat{O}_f = \sum_x (-1)^{f(x)} |x\rangle\langle x|, \quad U_s = H^{\otimes n} (2|0\dots 0\rangle\langle 0\dots 0| - I) H^{\otimes n} = H^{\otimes n} U_{|0\rangle^\perp} H^{\otimes n}.$$

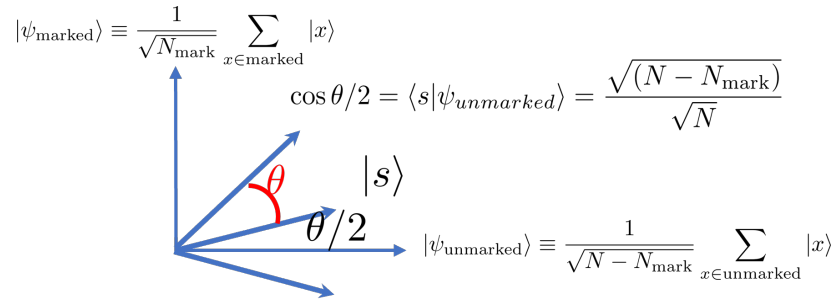


FIG. 5. Illustration of the geometric picture of the Grover's search algorithm.

The algorithm iteratively applies $\hat{G}$ to an initial state

$$|\psi_{\text{ini}}\rangle = H^{\otimes n}|0 \dots 0\rangle.$$

With such a picture, we can generalize the above form

$$\hat{G}_A = A U_{|0\rangle^\perp} A^{-1} \hat{O}_f = U_{|\psi\rangle^\perp} \hat{O}_f.$$

The initial state is generated by A ,

$$|\psi\rangle = A|0 \dots 0\rangle = \sin(\theta/2)|\psi_{\text{good}}\rangle + \cos(\theta/2)|\psi_{\text{bad}}\rangle,$$

where $|\psi_{\text{good}}\rangle$ is a superposition of all marked items and $|\psi_{\text{bad}}\rangle$ contains no marked item in the superposition. Note that $|00\dots 0\rangle$ can contain extra work qubits. The action of $\hat{G}_A$ is a rotation of θ in the 2D space spanned by $\{|\psi_{\text{good}}\rangle, |\psi_{\text{bad}}\rangle\}$, or equivalently, spanned by

$$\{|\psi\rangle, |\bar{\psi}\rangle \equiv \cos(\theta/2)|\psi_{\text{good}}\rangle - \sin(\theta/2)|\psi_{\text{bad}}\rangle\}.$$

Then the action of $\hat{G}_A$ on $|\psi\rangle$ leads to

$$(\hat{G}_A)^k |\psi\rangle = \sin(k\theta + \theta/2)|\psi_{\text{good}}\rangle + \cos(k\theta + \theta/2)|\psi_{\text{bad}}\rangle.$$

The goal is to get as close to $k\theta + \theta/2 = \pi/2$ for some integer k .

Note that similar to Grover's search, the operator $\hat{G}_A$ also has eigenvalues $e^{\pm i\theta}$, which, in principle, can be calculated from the so-called quantum phase estimation (to be covered in a later lecture).

Hadamard test and generalization. This part combines ideas from Hadamard test, amplitude amplification and quantum phase estimation; see, e.g., Section II of Ref. [20] for a summary. We have seen amplitude amplification, but we are not yet ready to discuss quantum phase estimation yet. Here, we will just illustrate the simplest scenario of the Hadamard test, shown in Eq. (4). Before the second Hadamard, the whole system is in

$$(|0\rangle|\psi_{\text{in}}\rangle + |1\rangle O|\psi_{\text{in}}\rangle)/\sqrt{2}. \quad (5)$$

Essentially, the Hadamard followed by measurement in 0/1 basis amounts to measuring in $+/-$ basis. Denote the outcome by $(-1)^s$, where s is 0 or 1 (corresponding to the final Z measurement outcome), the second qubit becomes

$$|\psi_{\text{out}}(s)\rangle = \frac{1}{2}(I + (-1)^s O)|\psi_{\text{in}}\rangle, \quad (6)$$

which is a projection onto the $+1$ or -1 eigenstate of O (assuming $O^2 = I$). This is a useful technique to project a state into eigenstates of an observable that squares to identity.

We will discuss quantum phase estimation after we learn quantum Fourier transform in a later unit.

VII. CONCLUDING REMARKS

In this unit, we have discussed the standard circuit-based quantum computation and introduced the Qiskit software developed by IBM.

It is a good time to check whether you have achieved the following Learning Outcomes:

After this Unit, (1) You'll be able to know elementary single-qubit and two-qubit quantum gates. (2) You'll be able to understand what quantum computation is and the specific quantum algorithm on searching. (3) You'll be able to get started in IBM Qiskit and run simple Jupyter notebooks of quantum circuits.

Suggested reading: N&C chap 4; KLM chap 4; Qb 1.4; 2.4, 2.5. A. Barenco et al., Elementary gates for quantum computation [21]. We note that N&C chap 4.5 has useful discussions on efficiency in approximating arbitrary single-qubit gates (from a discrete set of gates) and mentions the Solovay-Kitaev theorem that uses $O(\log^c(1/\epsilon))$ gates to an accuracy ϵ with $c \approx 2$, which is faster than a naive estimate $\Theta(1/\epsilon)$; see also their Appendix 3. It also discusses a very important issue on efficiency of approximating arbitrary unitary gates, which is generically hard. This conclusion can be obtained by ‘counting’ the ϵ -net on a $(2^{n+1} - 1)$ sphere in terms of $(2^{n+1} - 2)$ -sphere of radius ϵ , compared with the number of different states that m -gate circuits with g different types of gates (each on at most f qubits) can generate.

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- [1] J. L. Miller, Does quantum mechanics need imaginary numbers?, *Physics Today* **75**, 14 (2022).
 - [2] M.-O. Renou, D. Trillo, M. Weilenmann, T. P. Le, A. Tavakoli, N. Gisin, A. Acín, and M. Navascués, Quantum theory based on real numbers can be experimentally falsified, *Nature* **600**, 625 (2021).
 - [3] J. Bourgain and A. Gamburd, On the spectral gap for finitely-generated subgroups of $su(2)$, *Inventiones mathematicae* **171**, 83 (2008).
 - [4] I thank Prof. Greg Kuperberg for informing this and the following.
 - [5] N. J. Ross and P. Selinger, Optimal ancilla-free clifford+ t approximation of z-rotations., *Quantum Inf. Comput.* **16**, 901 (2016).
 - [6] A. Y. Kitaev, A. Shen, M. N. Vyalyi, *et al.*, *Classical and quantum computation*, Vol. 47 (American Mathematical Society Providence, RI, 2002).
 - [7] G. Kuperberg, Breaking the cubic barrier in the solovay-kitaev algorithm (2023), arXiv preprint arXiv:2306.13158.
 - [8] N. Yu, R. Duan, and M. Ying, Five two-qubit gates are necessary for implementing the toffoli gate, *Physical Review A* **88**, 010304 (2013).
 - [9] X.-Q. Zhou, T. C. Ralph, P. Kalasuwan, M. Zhang, A. Peruzzo, B. P. Lanyon, and J. L. O’Brien, Adding control to arbitrary unknown quantum operations, *Nature communications* **2**, 413 (2011).
 - [10] M. S. ANIS, Abby-Mitchell, H. Abraham, *et al.*, Qiskit: An open-source framework for quantum computing (2021).
 - [11] S. Bravyi and D. Maslov, Hadamard-free circuits expose the structure of the clifford group, *IEEE Transactions on Information Theory* **67**, 4546 (2021).
 - [12] S. X. Cui, D. Gottesman, and A. Krishna, Diagonal gates in the clifford hierarchy, *Phys. Rev. A* **95**, 012329 (2017).
 - [13] Z. He, L. Robitaille, and X. Tan, Permutation gates in the third level of the clifford hierarchy (2024), arXiv:2410.11818 [quant-ph].
 - [14] L. K. Grover, A fast quantum mechanical algorithm for database search, in *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing* (1996) pp. 212–219.
 - [15] L. K. Grover, Quantum mechanics helps in searching for a needle in a haystack, *Phys. Rev. Lett.* **79**, 325 (1997).
 - [16] L. K. Grover, Quantum computers can search rapidly by using almost any transformation, *Phys. Rev. Lett.* **80**, 4329 (1998).
 - [17] G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, Quantum amplitude amplification and estimation, *Contemporary Mathematics* **305**, 53 (2002).
 - [18] P. Høyer, Arbitrary phases in quantum amplitude amplification, *Phys. Rev. A* **62**, 052304 (2000).
 - [19] G.-L. Long, Grover algorithm with zero theoretical failure rate, *Physical Review A* **64**, 022307 (2001).
 - [20] J. Zhao, Y.-H. Zhang, C.-P. Shao, Y.-C. Wu, G.-C. Guo, and G.-P. Guo, Building quantum neural networks based on a swap test, *Phys. Rev. A* **100**, 012334 (2019).
 - [21] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, and H. Weinfurter, Elementary gates for quantum computation, *Phys. Rev. A* **52**, 3457 (1995).